```
=> d his

     (FILE 'HOME' ENTERED AT 14:47:12 ON 21 NOV 2002)

     FILE 'REGISTRY' ENTERED AT 14:53:28 ON 21 NOV 2002
               ACT TAT997P/A
               ---------
L1              STR
L2          102 SEA FILE=REGISTRY SSS FUL L1
               ---------
L3            1 S 157807-48-2
               ACT TAT997I/A
               ---------
L4           47 SEA FILE=REGISTRY ABB=ON  PLU=ON  (210108-85-3/BI OR 210108-86-
               ---------

     FILE 'HCAPLUS' ENTERED AT 14:54:19 ON 21 NOV 2002
               E AYLWARD J/AU

     FILE 'REGISTRY' ENTERED AT 14:56:06 ON 21 NOV 2002
L5          34 S L2 AND 2809.1.1/RID
L6          68 S L2 NOT L5

     FILE 'HCAPLUS' ENTERED AT 14:56:30 ON 21 NOV 2002
L7          28 S L5
               E AYLWARD J/AU
L8          29 S E15,E17,E20-23
L9           5 S L4 AND L8
L10         23 S L7 NOT L9
L11     576393 S IMMUN? OR? CANCER? OR ?TUMOR? OR ?CARCINOGEN? OR NEOPLAS? OR
L12          7 S L10 AND L11
L13          4 S L10(L)(DMA OR THU OR PKT OR PAC OR BAC)/RL
L14          0 S L12 AND L13
L15         12 S L10 NOT L12-13
L16          3 S L15 AND ?INFLAMM?
L17          9 S L15 NOT L16
L18         61 S L6
L19          7 S  L18(L)(DMA OR THU OR PKT OR PAC OR BAC)/RL
L20          4 S L19 AND (L11 OR ?INFLAMM?)
L21         13 S L18 AND (L11 OR ?INFLAMM?)
L22         16 S L19-21

     INDEX 'ADISALERTS, ADISINSIGHT, ADISNEWS, BABS, BIOBUSINESS, BIOCOMMERCE,
     BIOSIS, BIOTECHNO, CANCERLIT, CAPLUS, CBNB, CEN, CIN, CONFSCI, DDFB,
     DDFU, DGENE, DIOGENES, DRUGB, DRUGLAUNCH, DRUGMONOG2, DRUGNL, DRUGU,
     DRUGUPDATES, EMBAL, EMBASE, ESBIOBASE, ...' ENTERED AT 15:13:49 ON 21 NOV
     2002
               SEA ?INGENOL? OR ?INGENAN?
               ---------
                3*  FILE ADISALERTS
                3*  FILE ADISINSIGHT
                1*  FILE ADISNEWS
               64*  FILE BABS
                8*  FILE BIOBUSINESS
                0*  FILE BIOCOMMERCE
              198   FILE BIOSIS
               21   FILE BIOTECHNO
               79   FILE CANCERLIT
              267   FILE CAPLUS
                0*  FILE CBNB
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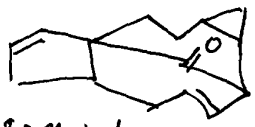
102 cpds from full file search

← cpds from relevant citations by applicant

34 cpds from STR search have this STR

related cpds



2809.1.1 is the ring identifier for this ring

28 cites for L5 cpds

cites from inventn search

7 cites

4 cites

Thu = therapy
PKT = pharmacokinetics
BAC = Biol. activity
PAC = pharmaco-dynamics
DMA = drug mech. of action
RL = Role

3 cites

9 cites - not related to therapy, etc

61 cites are related to the ingenane ring system

16 cites related to medical, etc

Index searching

Index searching

```
      1*  FILE CEN
      6*  FILE CONFSCI
     28*  FILE DDFB
     20*  FILE DDFU
      0*  FILE DGENE
      0*  FILE DIOGENES
     28*  FILE DRUGB
      0*  FILE DRUGLAUNCH
      0*  FILE DRUGMONOG2
      0*  FILE DRUGNL
     21*  FILE DRUGU
      0*  FILE DRUGUPDATES
      3*  FILE EMBAL
    149   FILE EMBASE
     37*  FILE ESBIOBASE
      8*  FILE FEDRIP
      7*  FILE IFIPAT
      0*  FILE INVESTEXT
     12*  FILE IPA
     24*  FILE JICST-EPLUS
      0*  FILE KOSMET
     28*  FILE LIFESCI
     99   FILE MEDLINE
    101   FILE NAPRALERT
     69*  FILE PASCAL
      1   FILE PHAR
      0*  FILE PHARMAML
      2*  FILE PROMT
    181   FILE SCISEARCH
      2*  FILE SYNTHLINE
    315   FILE TOXCENTER
     44   FILE USPATFULL
L23         QUE ?INGENOL? OR ?INGENAN?
            ---------

    FILE 'TOXCENTER, CAPLUS, BIOSIS, SCISEARCH, EMBASE, NAPRALERT, MEDLINE,
    CANCERLIT, PASCAL, BABS' ENTERED AT 15:16:13 ON 21 NOV 2002
L24        628 S EG1
L25        119 S EUPHORBIA FACTOR
L26          1 S L24 AND L25
L27       1522 S  ?INGENOL? OR ?INGENAN?
L28         61 S L27 AND (ANGELAT? OR MONOANGELAT?)
L30         36 S L28 AND (IMMUN? OR CANCER? OR ANTICANCER? OR TUMOR? OR ANTITU
L31          0 S L30 AND (STIMULAT?(3A)(IMMUN? OR INFLAMM?))
L32          2 S L30 AND (TREAT?(5A)(TUMOR? OR CANCER?))
L33         34 S L30 NOT L32
L34         10 DUP REM L33 (24 DUPLICATES REMOVED)
```

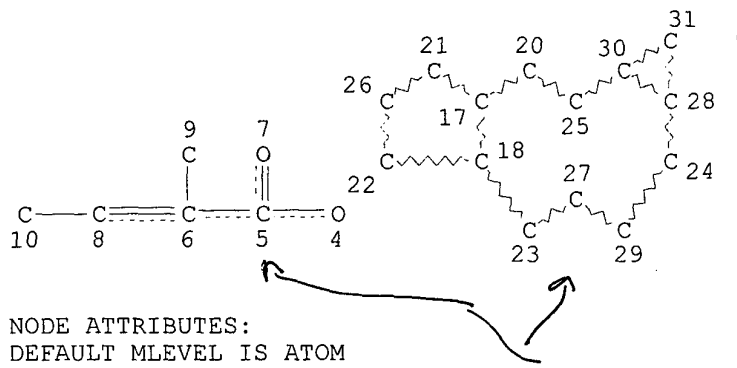
1 cite

2 cites

10 cites

STR for Reg / HCAPLUS search

=> d que l7
L1 STR



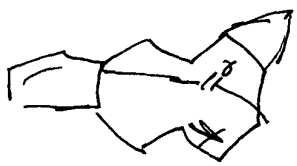
I drew this broadly since Appl. was claiming a derivative Fusion is allowed

NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

these 2 moieties can be joined in any manner

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 21

STEREO ATTRIBUTES: NONE
L2 102 SEA FILE=REGISTRY SSS FUL L1 102 cpds
L5 34 SEA FILE=REGISTRY ABB=ON PLU=ON L2 AND 2809.1.1/RID 34 cpds w/ ring ↓
L7 28 SEA FILE=HCAPLUS ABB=ON PLU=ON L5 28 cites



=> d ibib abs hitstr l12 1

L12 ANSWER 1 OF 7 HCAPLUS / COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2001:20788 HCAPLUS
DOCUMENT NUMBER: 135:136837
TITLE: Dietary cancer risk from conditional cancerogens (**tumor** promoters) in produce of livestock fed on species of spurge (Euphorbiaceae) V. Skin irritant and **tumor**-promoting diterpene ester toxins of the tigliane and ingenane type in the herbs Euphorbia nubica and Euphorbia helioscopia contaminating fodder of livestock
AUTHOR(S): Zayed, Salah M. A. D.; Farghaly, Madiha; Soliman, Soliman M.; Gotta, Hubert; Sorg, Bernd; Hecker, Erich
CORPORATE SOURCE: Laboratory of Organic Chemistry, Tahrir Street, National Research Center (NRC), Cairo, Dokki, Egypt
SOURCE: Journal of Cancer Research and Clinical Oncology (2001), 127(1), 40-47
CODEN: JCROD7; ISSN: 0171-5216
PUBLISHER: Springer-Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Irritant diterpene ester toxins were isolated from Euphorbia nubica and E. helioscopia, which are contaminants of the green fodder of livestock in Egypt. Fractionations of methanol exts. of aerial parts of both plants were monitored by the irritation unit on the mouse ear. Plant exts. were subjected to multiplicative distribution methods, yielding irritant hydrophilic fractions that were further purified by column chromatog. Final purifn. of the materials was achieved by TLC (silica gel) followed by HPLC, or by TLC alone. In this way, from E. nubica, five Euphorbia factors [Nu1 (I)-Nu5(V)] were isolated and characterized as short-chain polyfunctional diterpene esters of tigliane-type parent alcs. The two weak irritants I and III were triesters of 4-deoxy(4.alpha.)phorbol. II (R1 and R2 = COPh or COPr-i) was shown to be a triester of the stereoisomeric tigliane-type parent alc. 4-deoxyphorbol. Weak irritant IV probably is a positional isomer of II. V was characterized as a short-chain triester of 4,20-dideoxy-5.xi.-hydroxyphorbol. From E. helioscopia, six short- to medium-chain polyfunctional diterpene esters of the ingenane type, generally contg. unsatd. acids were obtained, i.e., four irritant esters of ingenol (Euphorbia factors H1, H2, H5, and H6) and two esters of 20-deoxyingenol (non-irritant Euphorbia substance HS4 (VI), and irritant Euphorbia factor H8). All irritant Euphorbia factors of the tigliane and ingenane diterpene ester type described in this investigation are considered to be more or less active **tumor** promoters, i.e., conditional (non-genotoxic) cancerogens. The Euphorbia factors assayed exhibited moderate (H1) to low (H8) relative **tumor**-promoting potency in comparison to the ingenane prototype DTE **tumor** promoter 3-TI.

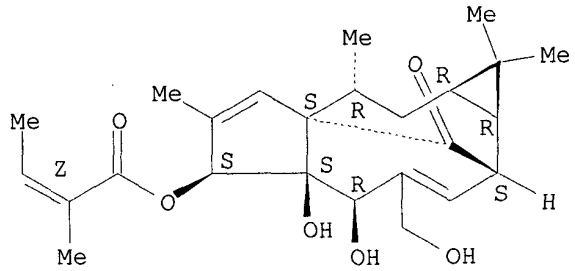
IT **75567-37-2P**, Euphorbia factor H1 **75567-38-3P**, Euphorbia factor H8 **91413-73-9P**, Euphorbia factor HS4
RL: ADV (Adverse effect, including toxicity); BOC (Biological occurrence); BSU (Biological study, unclassified); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)

(skin irritant and **tumor**-promoting diterpene ester toxins of tigliane and ingenane type in herbs Euphorbia nubica and Euphorbia helioscopia contaminating fodder of livestock)

RN 75567-37-2 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, (1aR,2S,5R,5aS,6S,8aS,9R,10aR)-1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-4-(hydroxymethyl)-1,1,7,9-tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, (2Z)- (9CI) (CA INDEX NAME)

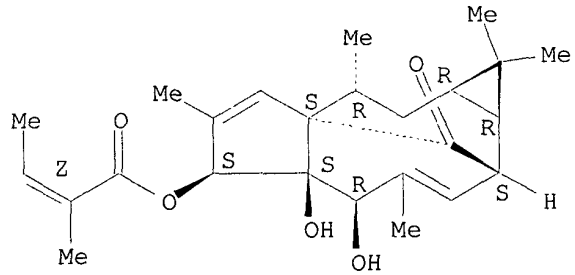
Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



RN 75567-38-3 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, (1aR,2S,5R,5aS,6S,8aS,9R,10aR)-1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-1,1,4,7,9-pentamethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, (2Z)- (9CI) (CA INDEX NAME)

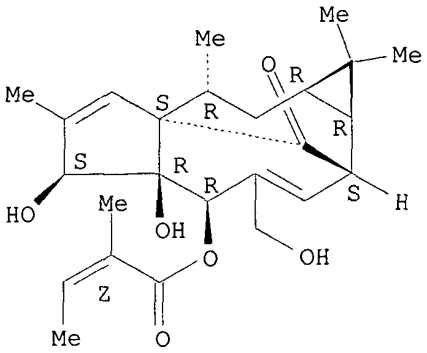
Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.



RN 91413-73-9 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, (1aR,2S,5R,5aR,6S,8aS,9R,10aR)-1a,2,5,5a,6,9,10,10a-octahydro-5a,6-dihydroxy-4-(hydroxymethyl)-1,1,7,9-tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-5-yl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

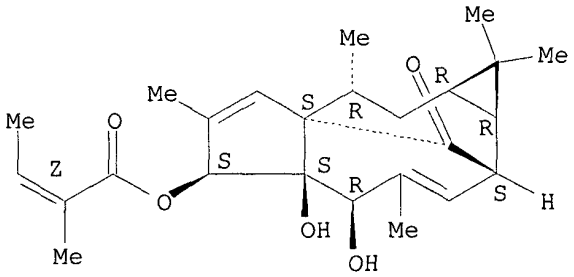


REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d ibib abs hitstr l12 2

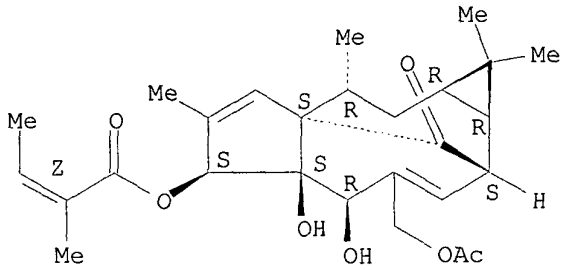
L12 ANSWER 2 OF 7 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1999:4251 HCAPLUS
DOCUMENT NUMBER: 130:34353
TITLE: Dietary cancer risk conditional cancerogens in produce of livestock fed on species of spurge (Euphorbiaceae). Part 1. Skin irritant and **tumor**-promoting ingenane-type diterpene esters in E. peplus, one of several herbaceous Euphorbia species contaminating fodder of livestock. [Erratum to document cited in CA129:312034]
AUTHOR(S): Zayed, Salah M. A. D.; Farghaly, Madiha; Taha, Hamby; Gotta, Hubert; Hecker, Erich
CORPORATE SOURCE: Laboratory Organic Chemistry, National Research Center, Cairo, Egypt
SOURCE: Journal of Cancer Research and Clinical Oncology (1998), 124(6), 351
CODEN: JCROD7; ISSN: 0171-5216
PUBLISHER: Springer-Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
AB On page 135, in Table 2, the words "Low" in the last column should read "Medium"; the complete column is reprinted.
IT **75567-38-3P 82425-35-2P 88262-86-6P 91413-73-9P**
RL: ADV (Adverse effect, including toxicity); BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(skin irritant and **tumor**-promoting ingenane-type diterpene esters in Euphorbia (Erratum))
RN 75567-38-3 HCAPLUS
CN 2-Butenoic acid, 2-methyl-, (1aR,2S,5R,5aS,6S,8aS,9R,10aR)-1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-1,1,4,7,9-pentamethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.



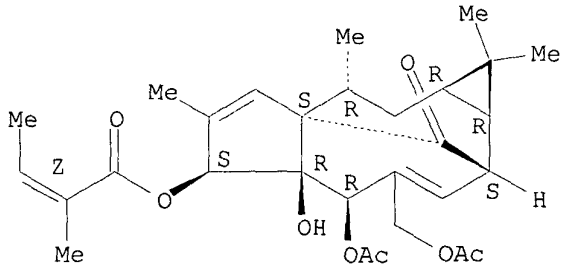
RN 82425-35-2 HCAPLUS
CN 2-Butenoic acid, 2-methyl-, (1aR,2S,5R,5aS,6S,8aS,9R,10aR)-4-[(acetyloxy)methyl]-1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-1,1,7,9-tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



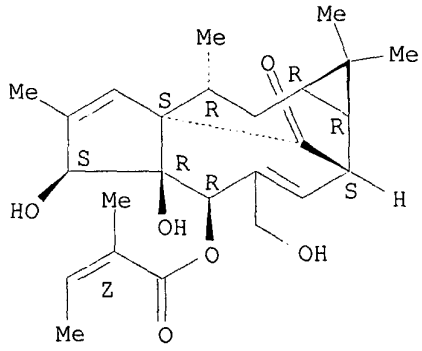
RN 88262-86-6 HCAPLUS
CN 2-Butenoic acid, 2-methyl-, (1aR,2S,5R,5aR,6S,8aS,9R,10aR)-5-(acetyloxy)-4-[(acetyloxy)methyl]-1a,2,5,5a,6,9,10,10a-octahydro-5a-hydroxy-1,1,7,9-tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



RN 91413-73-9 HCAPLUS
CN 2-Butenoic acid, 2-methyl-, (1aR,2S,5R,5aR,6S,8aS,9R,10aR)-1a,2,5,5a,6,9,10,10a-octahydro-5a,6-dihydroxy-4-(hydroxymethyl)-1,1,7,9-tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-5-yl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



=> d ibib abs hitstr l12 3

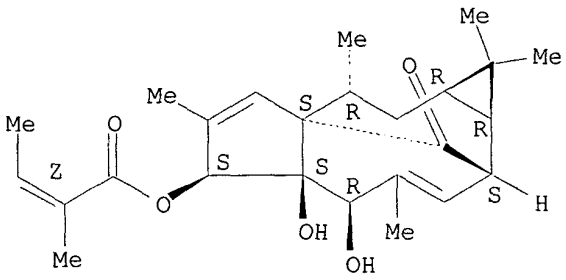
L12 ANSWER 3 OF 7 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1998:577094 HCAPLUS
DOCUMENT NUMBER: 129:312034
TITLE: Dietary cancer risk conditional cancerogens in produce of livestock fed on species of spurge (Euphorbiaceae). Part 1. Skin irritant and **tumor**-promoting ingenane-type diterpene esters in E. peplus, one of several herbaceous Euphorbia species contaminating fodder of livestock
AUTHOR(S): Zayed, Salah M. A. D.; Farghaly, Madiha; Taha, Hamdy; Gotta, Hubert; Hecker, Erich
CORPORATE SOURCE: Laboratory Organic Chemistry, National Research Center, Cairo, Egypt
SOURCE: Journal of Cancer Research and Clinical Oncology (1998), 124(3/4), 131-140
CODEN: JCROD7; ISSN: 0171-5216
PUBLISHER: Springer-Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Several herbaceous plants of the genus Euphorbia, widespread as weeds and contaminants of livestock fodder, were identified botanically and exts. of their aerial parts were tested for irritancy on the mouse ear. As compared to a std. probe of croton oil, the exts. of E. peplus, E. nubica, and E. helioscopia displayed irritancy. The most active ext. (that from E. peplus) was investigated by a fractionation procedure monitored by the mouse ear assay, and 5 molecularly uniform irritant E. factors Pe1-Pe5 were identified as diterpene ester-type toxins. Together these factors comprise at least 11 ppm in the aerial parts. They were characterized individually to carry the diterpene parent alcs. ingenol, 20-deoxyingenol, and 20-deoxyingenol-6.alpha.,7.alpha.-epoxide. The irritancy of the aerial plant parts was caused mainly by the E. factors Pe1 and Pe2 together. Upon chronic administration of these irritants and hyperplasiogens as principal cancerogenic risk factors in the mouse skin initiation/promotion bioassay, Pe1 and Pe2 were established as **tumor** promoters.

IT **75567-38-3P 82425-35-2P 88262-86-6P 91413-73-9P**
RL: ADV (Adverse effect, including toxicity); BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(skin irritant and **tumor**-promoting ingenane-type diterpene esters in Euphorbia)

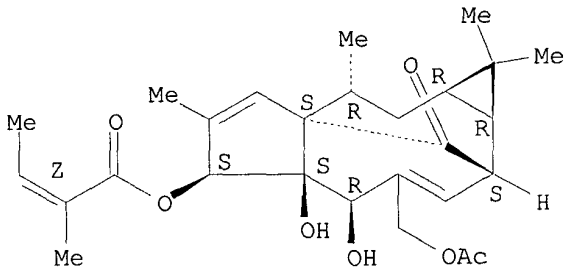
RN 75567-38-3 HCAPLUS
CN 2-Butenoic acid, 2-methyl-, (1aR,2S,5R,5aS,6S,8aS,9R,10aR)-1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-1,1,4,7,9-pentamethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.



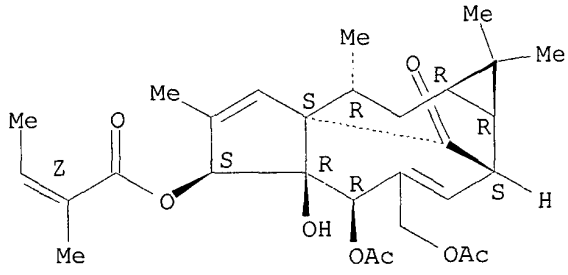
RN 82425-35-2 HCAPLUS
CN 2-Butenoic acid, 2-methyl-, (1aR,2S,5R,5aS,6S,8aS,9R,10aR)-4-[(acetyloxy)methyl]-1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-1,1,7,9-tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



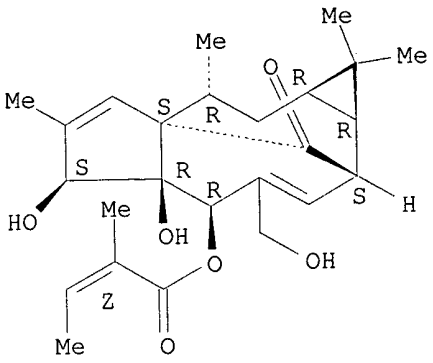
RN 88262-86-6 HCAPLUS
CN 2-Butenoic acid, 2-methyl-, (1aR,2S,5R,5aR,6S,8aS,9R,10aR)-5-(acetyloxy)-4-[(acetyloxy)methyl]-1a,2,5,5a,6,9,10,10a-octahydro-5a-hydroxy-1,1,7,9-tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



RN 91413-73-9 HCAPLUS
CN 2-Butenoic acid, 2-methyl-, (1aR,2S,5R,5aR,6S,8aS,9R,10aR)-1a,2,5,5a,6,9,10,10a-octahydro-5a,6-dihydroxy-4-(hydroxymethyl)-1,1,7,9-tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-5-yl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



=> d ibib abs hitstr l12 4

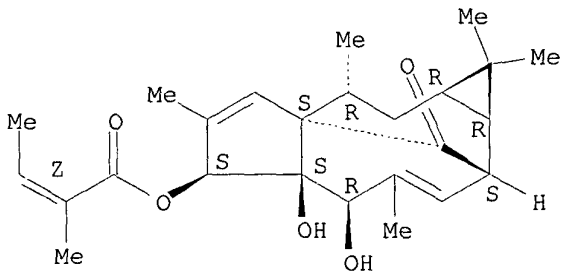
L12 ANSWER 4 OF 7 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1998:577085 HCAPLUS
DOCUMENT NUMBER: 129:274976
TITLE: Dietary cancer risk from conditional cancerogens in produce of livestock fed on species of spurge (Euphorbiahceae). Part 3. Milk of lactating goats fed on the skin irritant herb Euphorbia peplus is polluted by **tumor** promoters of the ingenane diterpene ester type
AUTHOR(S): Zayed, Salah M. A. D.; Farghaly, Madiha; Taha, Hamdy; Gminski, Richard; Hecker, Erich
CORPORATE SOURCE: Laboratory Organic Chemistry, National Research Center, Cairo, Egypt
SOURCE: Journal of Cancer Research and Clinical Oncology (1998), 124(6), 301-306
CODEN: JCROD7; ISSN: 0171-5216
PUBLISHER: Springer-Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Poisonous milk was investigated from lactating goats fed exptl. on aerial parts of the herb E. peplus. In milk exts., weakly irritant in the mouse-ear assay, diterpene ester toxins of the ingenane structural type (Euphorbia factor Pe 1, 2, 4) were detected by HPLC. The toxins were identical to diterpene esters in the aerial parts. Milk collected 15 days after cessation of the feeding was completely toxin free. The non-toxic parent alc. ingenol was also detected in the milk but not in the plant indicating a metabolic generation by the goats. The authors suggest a possible mechanism for the development of esophageal cancer in certain areas in Iran.

IT **75567-38-3 82425-35-2 91413-73-9**
RL: POL (Pollutant); OCCU (Occurrence)
(milk of lactating goats fed on the skin irritant herb Euphorbia peplus is polluted by **tumor** promoters of the ingenane diterpene ester type)

RN 75567-38-3 HCAPLUS
CN 2-Butenoic acid, 2-methyl-, (1aR,2S,5R,5aS,6S,8aS,9R,10aR)-1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-1,1,4,7,9-pentamethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, (2Z)- (9CI) (CA INDEX NAME)

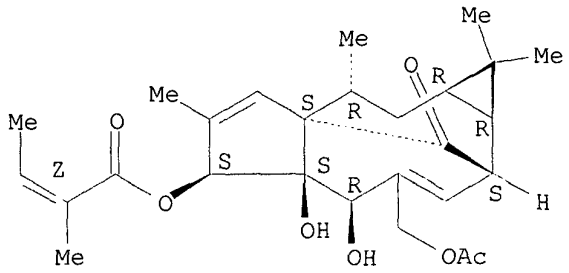
Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.



RN 82425-35-2 HCAPLUS
CN 2-Butenoic acid, 2-methyl-, (1aR,2S,5R,5aS,6S,8aS,9R,10aR)-4-

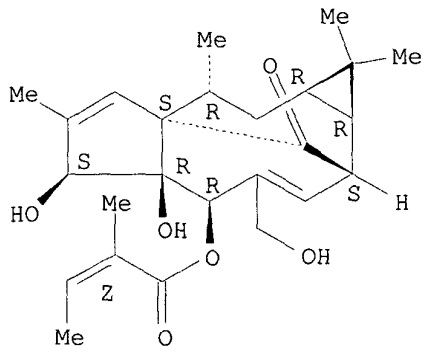
[(acetyloxy)methyl]-1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-1,1,7,9-tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



RN 91413-73-9 HCAPLUS
CN 2-Butenoic acid, 2-methyl-, (1aR,2S,5R,5aR,6S,8aS,9R,10aR)-1a,2,5,5a,6,9,10,10a-octahydro-5a,6-dihydroxy-4-(hydroxymethyl)-1,1,7,9-tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-5-yl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



=> d ibib abs hitstr l12 5

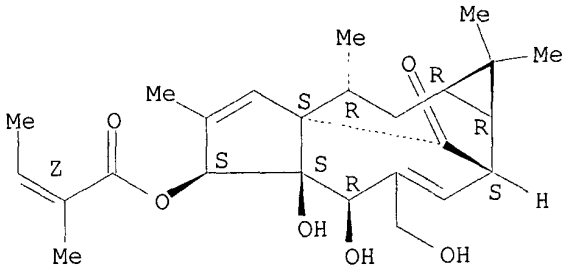
L12 ANSWER 5 OF 7 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1984:507324 HCAPLUS
DOCUMENT NUMBER: 101:107324
TITLE: On the active principles of the Euphorbiaceae, IX. Ingenane type diterpene esters from five Euphorbia species
AUTHOR(S): Gotta, H.; Adolf, W.; Opferkuch, H. J.; Hecker, E.
CORPORATE SOURCE: Inst. Biochem., Dtsch. Krebsforschungszent., Heidelberg, D-6900, Fed. Rep. Ger.
SOURCE: Zeitschrift fuer Naturforschung, Teil B: Anorganische Chemie, Organische Chemie (1984), 39B(5), 683-94
CODEN: ZNBAD2; ISSN: 0340-5087
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Investigation of E. antiquorum, E. helioscopia, E. palustris, E. peplus, and E. quadrialata for irritant and **tumor**-promoting constituents afforded several new ingenane diterpene esters derived from the parent alcs. ingenol and 20-deoxyingenol and from the hitherto unknown 20-deoxy-16-hydroxyingenol and 20-deoxy-13,16-dihydroxyingenol. The irritant activities of the natural compds. are reported, together with some aspects on structure activity relationships.

IT **75567-37-2 82425-35-2 88262-77-5**
91413-73-9
RL: BIOL (Biological study)
(from Euphorbia species)

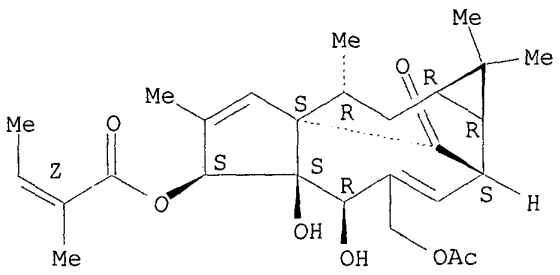
RN 75567-37-2 HCAPLUS
CN 2-Butenoic acid, 2-methyl-, (1aR,2S,5R,5aS,6S,8aS,9R,10aR)-1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-4-(hydroxymethyl)-1,1,7,9-tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



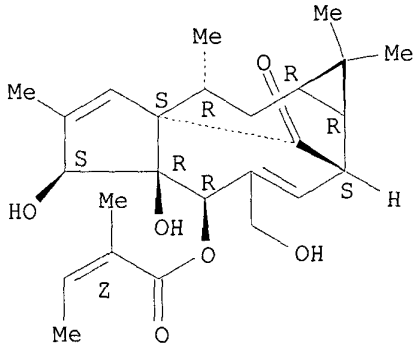
RN 82425-35-2 HCAPLUS
CN 2-Butenoic acid, 2-methyl-, (1aR,2S,5R,5aS,6S,8aS,9R,10aR)-4-[(acetyloxy)methyl]-1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-1,1,7,9-tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



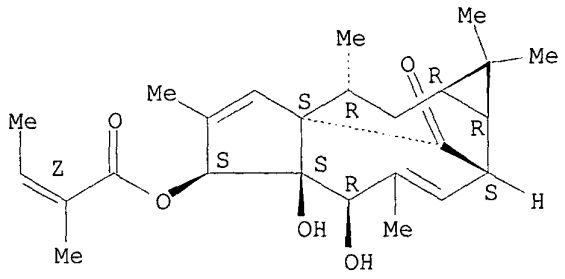
RN 88262-77-5 HCAPLUS
RN 91413-73-9 HCAPLUS
CN 2-Butenoic acid, 2-methyl-, (1aR,2S,5R,5aR,6S,8aS,9R,10aR)-1a,2,5,5a,6,9,10,10a-octahydro-5a,6-dihydroxy-4-(hydroxymethyl)-1,1,7,9-tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-5-yl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



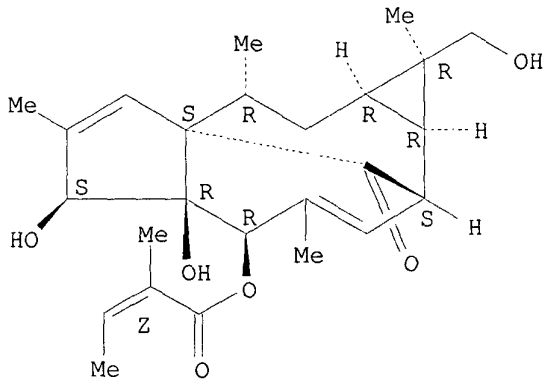
IT **75567-38-3P 88262-92-4P 91413-81-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 75567-38-3 HCAPLUS
CN 2-Butenoic acid, 2-methyl-, (1aR,2S,5R,5aS,6S,8aS,9R,10aR)-1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-1,1,4,7,9-pentamethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.

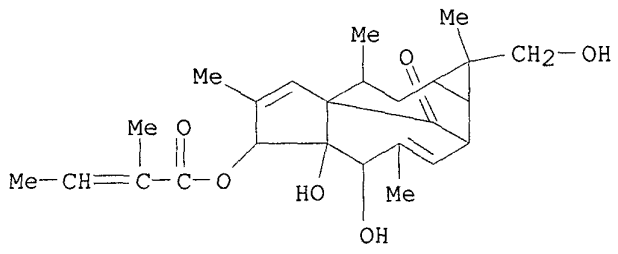


RN 88262-92-4 HCAPLUS
CN 2-Butenoic acid, 2-methyl-, 1a,2,5,5a,6,9,10,10a-octahydro-5a,6-dihydroxy-1-(hydroxymethyl)-1,4,7,9-tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-5-yl ester, [1R-[1.alpha.,1a.beta.,2.alpha.,5.alpha.(Z),5a.alpha.,6.alpha.,8a.beta.,9.beta.,10a.beta.]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

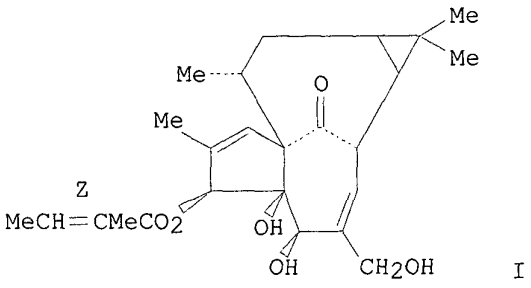


RN 91413-81-9 HCAPLUS
CN 2-Butenoic acid, 2-methyl-, 1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-1-(hydroxymethyl)-1,4,7,9-tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, [1S-[1.alpha.,1a.alpha.,2.beta.,5.beta.,5a.beta.,6.beta.(Z),8a.alpha.,9.alpha.,10a.alpha.]]- (9CI) (CA INDEX NAME)



=> d ibib abs hitstr l12 6

L12 ANSWER 6 OF 7 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1984:12496 HCAPLUS
DOCUMENT NUMBER: 100:12496
TITLE: 3-O-Angeloylingenol, the toxic and skin irritant factor from latex of Euphorbia antiquorum L. (Euphorbiaceae) and from a derived Thai purgative and anthelimintic (vermifuge) drug
AUTHOR(S): Adolf, W.; Chanai, S.; Hecker, E.
CORPORATE SOURCE: Inst. Biochem., Dtsch. Krebsforschungszent., Heidelberg, D-6900, Fed. Rep. Ger.
SOURCE: Journal of the Science Society of Thailand (1983), 9(2), 81-8
CODEN: VKSTDB; ISSN: 0303-8122
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



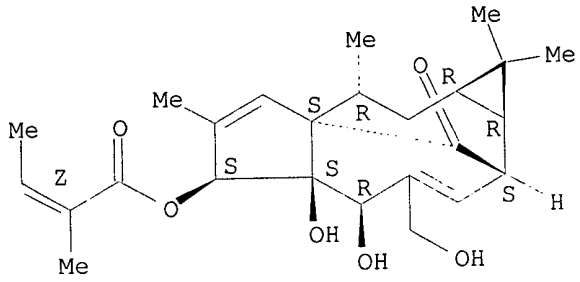
I

AB From a latex of E. antiquorum, as well as from the purgative and anthelmintic (vermifuge) Thai drug yang Sa-Lad-Dai (dried, powd. latex), the highly skin irritant and toxic Euphorbia factor An1 3-O-angeloylingenol (I) [**75567-37-2**] was isolated by combination of countercurrent distributions and chromatog. Because of the acute toxicity of I and of the possible risk of **cocarcinogenesis** by **tumor** promotion, utilization of drugs made up from dried or fresh latex as practiced in Thailand in purgatives and vermifuges should be abandoned.

IT **75567-37-2**
RL: BIOL (Biological study)
(of Euphorbia antiquorum latex, skin irritation from)

RN 75567-37-2 HCAPLUS
CN 2-Butenoic acid, 2-methyl-, (1aR,2S,5R,5aS,6S,8aS,9R,10aR)-1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-4-(hydroxymethyl)-1,1,7,9-tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.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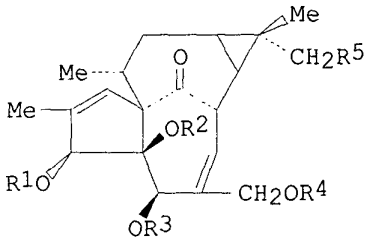
=> d ibib abs hitstr l12 7

L12 ANSWER 7 OF 7 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1983:12688 HCAPLUS
DOCUMENT NUMBER: 98:12688
TITLE: On the active principles of the spurge family (Euphorbiaceae). IV. Skin irritant and **tumor** promoting diterpene esters from Euphorbia ingens E. Mey
AUTHOR(S): Opferkuch, H. J.; Hecker, E.
CORPORATE SOURCE: Inst. Biochem., Dtsch. Krebsforschungszent., Heidelberg, D-6900/1, Fed. Rep. Ger.
SOURCE: Journal of Cancer Research and Clinical Oncology (1982), 103(3), 255-68
CODEN: JCROD7; ISSN: 0171-5216
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

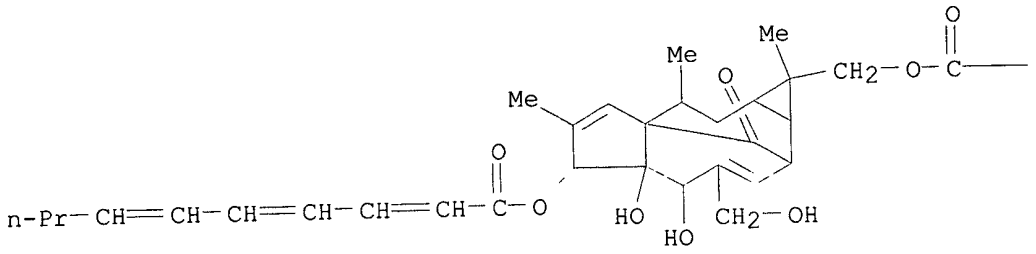
AB The irritant and **tumor**-promoting principles of the latex of Euphorbia ingens were isolated together with several nonirritant compds. The Euphorbia factor I1 [52557-26-3], I5 [**52557-27-4**], and I6 [52557-28-5] are esters of ingenane-type polyfunctional diterpene alcs. (I). Euphorbia factor I1 is characterized as the 3-hexadecanoate of I and Euphorbia factor I6 as the 3-deca-2.4.6-trienoic acid ester of I. Euphorbia factor I5 is the 16-angelate-3-deca-2.4.6-trienoate of 16-hydroxyingenol. Nonirritant diterpenes of the latex are I2 [39071-33-5], the ingenol-20-hexadecanoate - an isomer of Euphorbia factor I1 - and I4, the 3.7.12-triacetate-8-nicotinate of the macrocyclic lathyrane-type polyfunctional diterpene alc. ingol. The diterpene alcs. ingenol and 16-hydroxyingenol are inactive as irritants and **tumor** promoters of mouse skin. Compared to croton oil factor A1, the Euphorbia factor I1 exhibits .apprx.1/10 of the irritant and **tumor** -promoting activity in mouse skin. I1 shows no reasonable **tumorigenic** activity. Compared with I1, Euphorbia factors I5 and I6 are more potent irritants and less potent **tumor** promoters.

IT **52557-27-4**
RL: BIOL (Biological study)
(**neoplasm** promotion and skin irritation by)

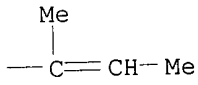
RN 52557-27-4 HCAPLUS

CN 2,4,6-Decatrienoic acid, (1S,1aR,2S,5R,5aR,6S,8aS,9R,10aR)-1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-4-(hydroxymethyl)-1,7,9-trimethyl-1-[[[(2Z)-2-methyl-1-oxo-2-butenyl]oxy]methyl]-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



=> d ibib abs hitstr l13 1

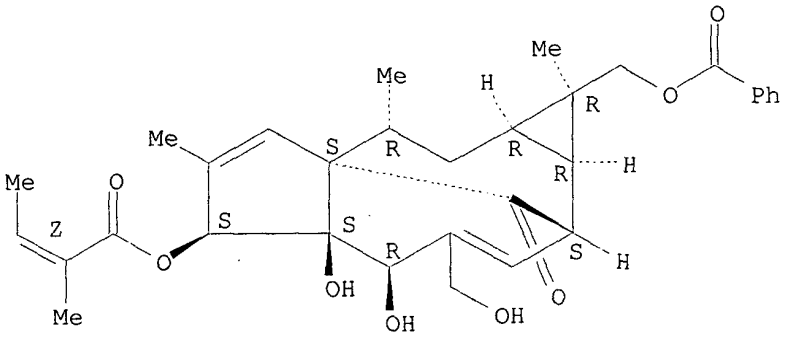
L13 ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1998:223682 HCAPLUS
DOCUMENT NUMBER: 129:321
TITLE: Comparative analysis of the vascular actions of diterpenes isolated from Euphorbia canariensis
AUTHOR(S): Miranda, Francisco J.; Alabadi, Jose A.; Orti, Marta; Centeno, Jose M.; Pinon, Marta; Yuste, Alberto; Sanz-Cervera, Juan F.; Marco, J. Alberto; Alborch, Enrique
CORPORATE SOURCE: Department of Physiology, University of Valencia, Valencia, E-46100, Spain
SOURCE: Journal of Pharmacy and Pharmacology (1998), 50(2), 237-241
CODEN: JPPMAB; ISSN: 0022-3573
PUBLISHER: Royal Pharmaceutical Society of Great Britain
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The effects of 2,3-diepiingol 7,12-diacetate-8-isobutyrate (I), ingenol-3-angelate-17-benzoate (II), ingenol-3-angelate-17-benzoate-20-acetate (III) and 3,5,7,8,9,15-hexahydroxyjatropha-6(17),11-dien-14-one-5,8-bis(2-methylbutyrate)-7-(2-methylpropionate) (IV), isolated from E. canariensis, on the isometric tension developed by isolated rabbit basilar and carotid arteries were studied. Concn.-response curves to these compds. were obtained cumulatively in both arteries at resting tension and active tone (KCl, 50 mM). At resting tension a concn.-dependent contraction was induced by the four compds. In the basilar artery the order of potency was III = I > II = IV, without significant differences between Emax values. In the carotid artery the order of potency was III > II = I = IV and there were no significant differences between the Emax (max. effect) values of I-III, all of which were higher than that of IV. In pre-contracted basilar artery I-III induced concn.-dependent relaxation and IV was almost ineffective; the order of potency was III > II = I without significant differences between Emax values. In the carotid artery with active tone the four compds. induced further contractions; the order of potency was III > II = IV > I without significant differences between Emax values. These results show that the four diterpenes are potent active substances in rabbit basilar and carotid arteries and that there are regional differences between their action. All four compds. contract basilar and carotid arteries at resting tension. I-III relax pre-contracted basilar artery but not carotid artery.

IT **83983-93-1 192825-63-1**
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); BIOL (Biological study)
(vascular actions of diterpenes isolated from Euphorbia canariensis)

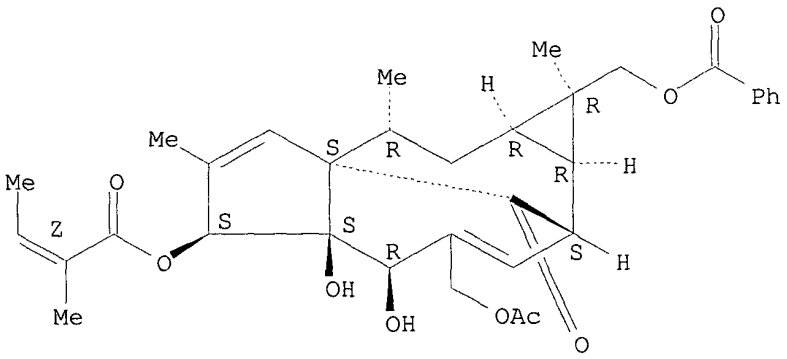
RN 83983-93-1 HCAPLUS
CN 2-Butenoic acid, 2-methyl-, (1R,1aR,2S,5R,5aS,6S,8aS,9R,10aR)-1-[(benzoyloxy)methyl]-1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-4-(hydroxymethyl)-1,7,9-trimethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 192825-63-1 HCAPLUS
CN 2-Butenoic acid, 2-methyl-, (1R,1aR,2S,5R,5aS,6S,8aS,9R,10aR)-4-[(acetyloxy)methyl]-1-[(benzoyloxy)methyl]-1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-1,7,9-trimethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



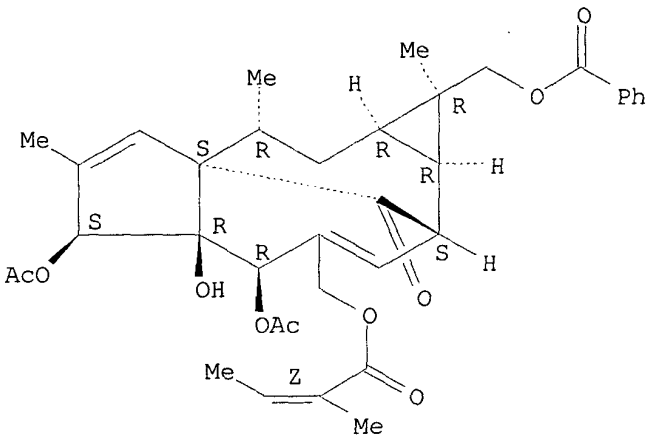
=> d ind l13 1

L13 ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2002 ACS
CC 1-8 (Pharmacology)
ST Euphorbia diterpene vascular activity; ingenol analog Euphorbia vascular activity; jatrophane analog Euphorbia vascular activity; vasoconstrictor Euphorbia diterpene
IT Euphorbia canariensis
Vasoconstrictors
(vascular actions of diterpenes isolated from Euphorbia canariensis)
IT Diterpenes
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); BIOL (Biological study)
(vascular actions of diterpenes isolated from Euphorbia canariensis)
IT **83983-93-1 192825-63-1** 207346-95-0 207346-96-1
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); BIOL (Biological study)
(vascular actions of diterpenes isolated from Euphorbia canariensis)

=> d ibib abs hitstr ind l13 2

L13 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1997:578751 HCAPLUS
DOCUMENT NUMBER: 127:257318
TITLE: Analysis of the vascular effects of an ingenol derivative isolated from Euphorbia canariensis
AUTHOR(S): Miranda, Francisco J.; Alabadi, Jose A.; Pinon, Marta; Orti, Marta; Centeno, Jose M.; Yuste, Alberto; Sanz-Cervera, Juan F.; Marco, J. Alberto; Alborch, Enrique
CORPORATE SOURCE: Department of Physiology, University of Valencia, Valencia, E-46100, Spain
SOURCE: Pharmaceutical Sciences (1997), 3(2), 113-116
CODEN: PHSCFB; ISSN: 1356-6881
PUBLISHER: Royal Pharmaceutical Society of Great Britain
DOCUMENT TYPE: Journal
LANGUAGE: English
AB We have analyzed the effects of 3-O-[(Z)-2-methyl-2-butenoyl]-5,20-O-diacetyl-17-O-benzoyl-17-hydroxyingenol (MBDH), an ingenol deriv. isolated from Euphorbia canariensis, on isometric tension developed by isolated rabbit basilar and carotid arteries. MBDH concn.-response curves (10-8 - 3 .times. 10-5 M) were obtained cumulatively in precontracted (KCl, 50 mM) arteries. In basilar artery, MBDH induced a concn.-dependent relaxation that was not modified by incubation with NG-nitro-L-arginine (L-NOARG) (10-5 M) or indomethacin (10-5 M). In carotid artery, a slight relaxant response to MBDH was obsd. at higher concns., which turned into contraction in the presence of either indomethacin or L-NOARG. These results suggest that MBDH has a relaxant action on rabbit basilar and carotid arteries. Nitric oxide and prostacyclin mediate this relaxant action in carotid artery but do not participate in the response obtained in basilar artery.
IT **192825-66-4**
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); BIOL (Biological study)
(vascular effects of an ingenol deriv. isolated from Euphorbia canariensis)
RN 192825-66-4 HCAPLUS
CN 2-Butenoic acid, 2-methyl-, 5,6-bis(acetyloxy)-[1-[(benzoyloxy)methyl]-1a,2,5,5a,6,9,10,10a-octahydro-5a-hydroxy-1,7,9-trimethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-4-yl]methyl ester, [1R-[1.alpha.,1a.beta.,2.alpha.,4(Z),5.alpha.,5a.alpha.,6.alpha.,8a.beta.,9.beta.,10a.beta.]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



CC 1-8 (Pharmacology)
ST Euphorbia ingenol deriv vasorelaxant prostacyclin NO
IT Euphorbia canariensis
Vasodilators
(vascular effects of an ingenol deriv. isolated from Euphorbia canariensis)
IT **192825-66-4**
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); BIOL (Biological study)
(vascular effects of an ingenol deriv. isolated from Euphorbia canariensis)
IT 10102-43-9, Nitric oxide, biological studies 35121-78-9, Prostacyclin
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(vascular effects of an ingenol deriv. isolated from Euphorbia canariensis)

=> d ibib abs hitstr ind l13 3

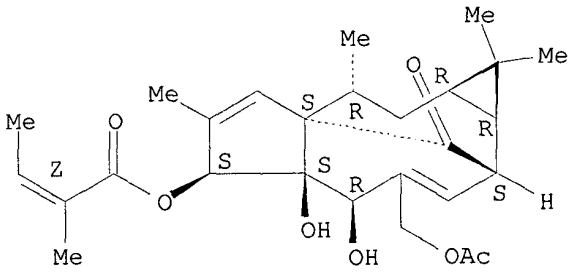
L13 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1989:454160 HCAPLUS
DOCUMENT NUMBER: 111:54160
TITLE: Toxic diterpenes from Euphorbia trigona (saiunkaku: an indoor foliage plant in Japan)
AUTHOR(S): Tada, Masahiro; Seki, Hiromichi
CORPORATE SOURCE: Lab. Bio-Org. Chem., Tokyo Univ. Agric. Technol., Tokyo, 183, Japan
SOURCE: Agricultural and Biological Chemistry (1989), 53(2), 425-30
CODEN: ABCHA6; ISSN: 0002-1369
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Three ingenol esters, displaying piscicidal activity, and an ingol ester were isolated from E. trigona. Their structures were unambiguously elucidated by means of IR, 1H- and 13C-NMR, and mass spectral data.

IT **82425-35-2 92998-75-9**
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); BIOL (Biological study)
(from Euphorbia trigona, isolation and piscicidal activity of)

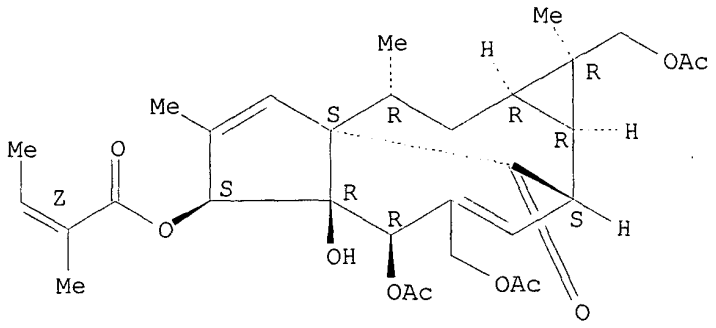
RN 82425-35-2 HCAPLUS
CN 2-Butenoic acid, 2-methyl-, (1aR,2S,5R,5aS,6S,8aS,9R,10aR)-4-[(acetyloxy)methyl]-1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-1,1,7,9-tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



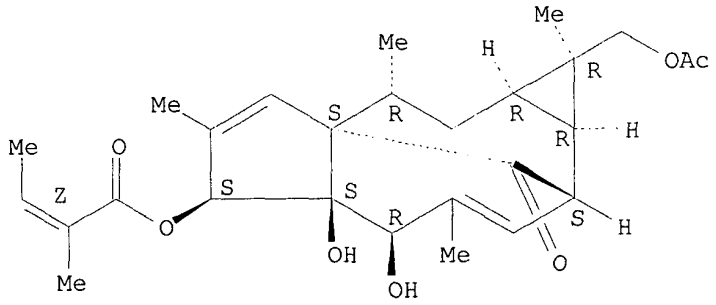
RN 92998-75-9 HCAPLUS
CN 2-Butenoic acid, 2-methyl-, 5-(acetyloxy)-1,4-bis[(acetyloxy)methyl]-1a,2,5,5a,6,9,10,10a-octahydro-5a-hydroxy-1,7,9-trimethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, [1R-[1.alpha.,1a.beta.,2.alpha.,5.alpha.,5a.alpha.,6.alpha.(Z),8a.beta.,9.beta.,10a.beta.]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



IT **121570-35-2**
RL: BIOL (Biological study)
(from Euphorbia trigona, isolation and structure and piscicidal activity of)
RN 121570-35-2 HCAPLUS
CN 2-Butenoic acid, 2-methyl-, (1R,1aR,2S,5R,5aS,6S,8aS,9R,10aR)-1-[(acetyloxy)methyl]-1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-1,4,7,9-tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



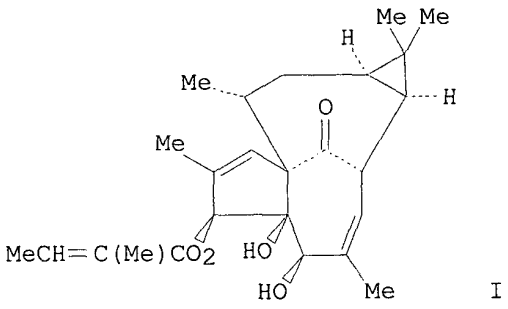
CC 11-1 (Plant Biochemistry)
Section cross-reference(s): 30
ST Euphorbia diterpene ingenol ingol ester piscicide
IT Euphorbia trigona
(ingenol and ingol esters from aerial parts of, isolation and structure and piscicidal activity of)
IT Piscicides
(ingenol esters from Euphorbia trigona as)
IT Diterpenes and Diterpenoids
RL: BIOL (Biological study)
(esters, from Euphorbia trigona, isolation and structure and piscicidal activity of)
IT **82425-35-2 92998-75-9**
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); BIOL (Biological study)
(from Euphorbia trigona, isolation and piscicidal activity of)
IT **121570-35-2**
RL: BIOL (Biological study)
(from Euphorbia trigona, isolation and structure and piscicidal

activity of)

IT 121570-36-3
RL: BIOL (Biological study)
(from Euphorbia trigona, isolation and structure and plant growth inhibitory activity of)

=> d ibib abs hitstr ind l13 4

L13 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1985:557302 HCAPLUS
DOCUMENT NUMBER: 103:157302
TITLE: Constituents of Egyptian Euphorbiaceae. Part 13. Biologically active diterpene esters from Euphorbia peplus
AUTHOR(S): Rizk, A. M.; Hammouda, F. M.; El-Missiry, M. M.; Radwan, H. M.; Evans, F. J.
CORPORATE SOURCE: Pharm. Sci. Lab., Natl. Res. Cent., Cairo, Egypt
SOURCE: Phytochemistry (Elsevier) (1985), 24(7), 1605-6
CODEN: PYTCAS; ISSN: 0031-9422
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

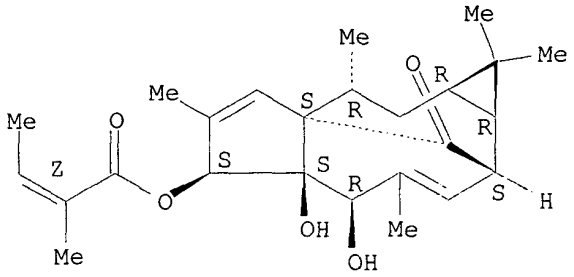
AB By means of partition and preparative TLC, 2 pro-inflammatory diterpene esters were isolated from E. peplus. These compds. were identified as 20-deoxyingenol 3-O-angelate, which exhibited an irritant dose (for 50% irritation) of 0.18 .mu.g on mouse skin, and the new ester ingenol 20-O-octanoate (I), which exhibited an irritant dose (for 50% irritation) of 1.0 .mu.g on mouse skin.

IT **75567-38-3P**
RL: PREP (Preparation)
(purifn. and inflammatory activity of, of Euphorbia peplus)

RN 75567-38-3 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, (1aR,2S,5R,5aS,6S,8aS,9R,10aR)-1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-1,1,4,7,9-pentamethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, (2Z)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.



CC 11-1 (Plant Biochemistry)
Section cross-reference(s): 4

ST Euphorbia terpene deoxyingenolangelate ingenoloctanoate; irritant terpene Euphorbia

IT Euphorbia peplus
(diterpene esters from)

IT Esters, biological studies
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); BIOL (Biological study)
(diterpenoid, inflammatory activity of, of Euphorbia peplus)

IT Diterpenes and Diterpenoids
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); BIOL (Biological study)
(esters, inflammatory activity of, of Euphorbia peplus)

IT Skin, toxic chemical and physical damage
(irritation, from Euphorbia peplus diterpene esters)

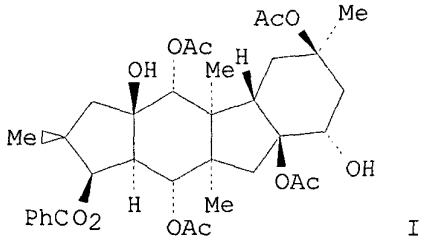
IT 30220-45-2P 54707-00-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

IT **75567-38-3P** 98649-87-7P
RL: PREP (Preparation)
(purifn. and inflammatory activity of, of Euphorbia peplus)

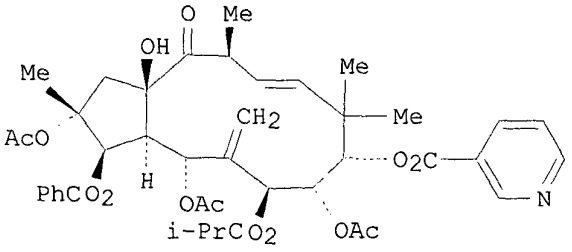
=> d ibib abs hitstr ind 1

L16 ANSWER 1 OF 3 HCAPLUS ?COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2000:310802 HCAPLUS
DOCUMENT NUMBER: 133:86701
TITLE: Diterpenoids from Euphorbia peplus
AUTHOR(S): Hohmann, Judit; Evanics, Ferenc; Berta, Laszlo; Bartok, Tibor
CORPORATE SOURCE: Department of Pharmacognosy, Albert Szent-Gyorgyi Medical University, Szeged, 6701, Hung.
SOURCE: Planta Medica (2000), 66(3), 291-294
CODEN: PLMEAA; ISSN: 0032-0943
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I



II

AB From a pro-**inflammatory** active ext. of Euphorbia peplus, two new diterpene polyesters I and II based on the pepluane and jatrophane skeletons were isolated, together with four known ingenane and jatrophane diterpenes. The structures were detd. on the basis of extensive NMR studies. Ingenol 3-angelate, which was obtained for the first time from this plant, is an irritant toxin with high activity.

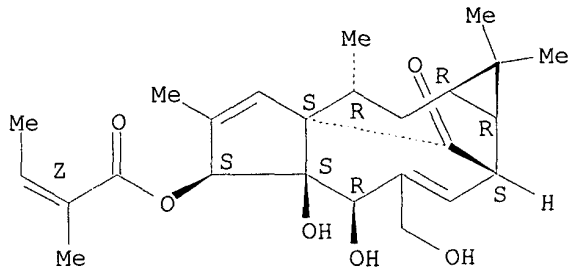
IT **75567-37-2 75567-38-3 91413-73-9**
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)
(diterpenoids from Euphorbia peplus)

RN 75567-37-2 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, (1aR,2S,5R,5aS,6S,8aS,9R,10aR)-1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-4-(hydroxymethyl)-1,1,7,9-tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, (2Z)- (9CI) (CA INDEX NAME)

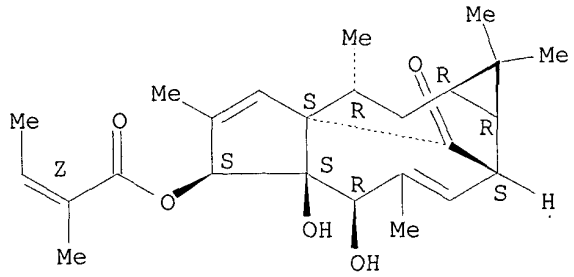
Absolute stereochemistry. Rotation (+).

Double bond geometry as shown.



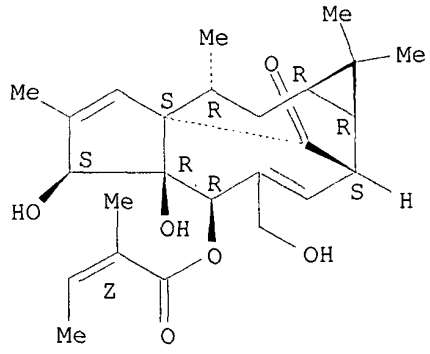
RN 75567-38-3 HCAPLUS
CN 2-Butenoic acid, 2-methyl-, (1aR,2S,5R,5aS,6S,8aS,9R,10aR)-1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-1,1,4,7,9-pentamethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.



RN 91413-73-9 HCAPLUS
CN 2-Butenoic acid, 2-methyl-, (1aR,2S,5R,5aR,6S,8aS,9R,10aR)-1a,2,5,5a,6,9,10,10a-octahydro-5a,6-dihydroxy-4-(hydroxymethyl)-1,1,7,9-tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-5-yl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

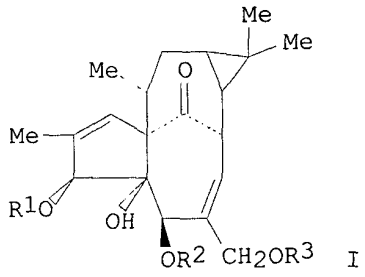


CC 11-1 (Plant Biochemistry)

Section cross-reference(s): 30
ST diterpenoid Euphorbia structure
IT Euphorbia peplus
New natural products
(diterpenoids from Euphorbia peplus)
IT Diterpenes
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(diterpenoids from Euphorbia peplus)
IT Molecular structure, natural product
(of diterpenoids from Euphorbia peplus)
IT **75567-37-2 75567-38-3 91413-73-9** 210108-85-3
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)
(diterpenoids from Euphorbia peplus)
IT 280553-67-5P 280553-68-6P
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(diterpenoids from Euphorbia peplus)
REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d ibib abs hitstr ind 2

L16 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1989:109558 HCAPLUS
DOCUMENT NUMBER: 110:109558
TITLE: Irritancy of ingenol esters from Euphorbia kamerunica
AUTHOR(S): Abo, K. A.
CORPORATE SOURCE: Coll. Med., Univ. Ibadan, Nigeria
SOURCE: Fitoterapia (1988), 59(3), 244-6
CODEN: FTRPAE; ISSN: 0367-326X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

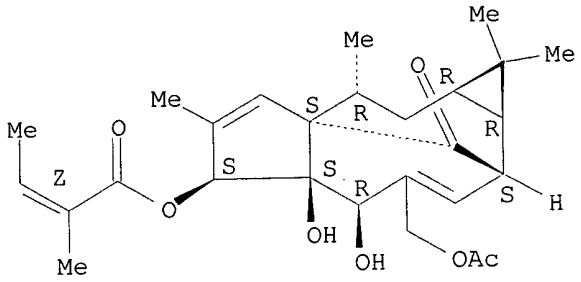
AB Six ingenol esters (I where R1 = H, dodecanoyl, decanoyl, Et, R2 = H, hexadienoyl, or octenoyl, and R3 = H or acetyl) showed irritant activity in the mouse ear assay. Monoesters were generally more potent than diesters. Monoesters exhibited chronic **inflammation** for .ltoreq.24 h. An ester function at C-3 or C-5 may be necessary for max. **inflammatory** response. A free C-20 primary etc. may be vital for max. activity and persistent **inflammation**.

IT **82425-35-2**
RL: BIOL (Biological study)
(skin irritation from)

RN 82425-35-2 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, (1aR,2S,5R,5aS,6S,8aS,9R,10aR)-4-[(acetyloxy)methyl]-1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-1,1,7,9-tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



CC 4-3 (Toxicology)
ST ingenol ester skin irritation
IT Skin, toxic chemical and physical damage
(ingenol esters irritation of)
IT Molecular structure-biological activity relationship
(skin-irritating, of ingenol esters)
IT 30220-46-3D, Ingenol, esters 67021-88-9 82425-34-1 **82425-35-2**
82438-00-4 82438-02-6 119000-34-9
RL: BIOL (Biological study)
(skin irritation from)

=> d ibib abs hitstr ind 3

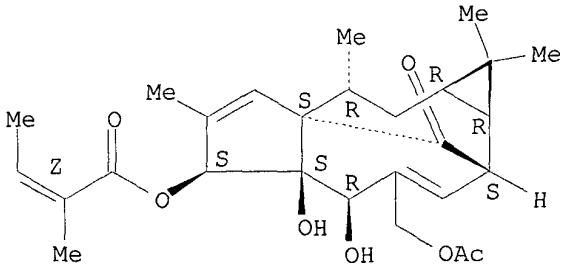
L16 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1982:452487 HCAPLUS
DOCUMENT NUMBER: 97:52487
TITLE: Ingenol esters from the pro-**inflammatory** fraction of Euphorbia kamerunica
AUTHOR(S): Abo, Kio A.; Evans, Fred J.
CORPORATE SOURCE: Dep. Pharmacogn., Sch. Pharm., London, WC1N 1AX, UK
SOURCE: Phytochemistry (1982), 21(3), 725-6
CODEN: PYTCAS; ISSN: 0031-9422
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A series of unstable mono- and diesters of the tetracyclic diterpene irigenol were isolated from the **proinflammatory** ether-sol. fraction of the latex of E. kamerunica by column and thin-layer chromatog. The monoesters were identified by spectroscopic methods and hydrolysis reactions as the 3-decanoate, 3-dodecanoate, 5-hexadienoate, and 5-octenoate, and the diesters as 20-acetylingenol-3-octenoate and -3-angelate.

IT **82425-35-2**
RL: BIOL (Biological study)
(from Euphorbia kamerunica)

RN 82425-35-2 HCAPLUS
CN 2-Butenoic acid, 2-methyl-, (1aR,2S,5R,5aS,6S,8aS,9R,10aR)-4-[(acetyloxy)methyl]-1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-1,1,7,9-tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



CC 11-1 (Plant Biochemistry)
Section cross-reference(s): 30
ST Euphorbia ingenol esters
IT Euphorbia kamerunica
(ingenol esters of)
IT Diterpenes and Diterpenoids
RL: BIOL (Biological study)
(ingenol esters, from Euphorbia kamerunica)
IT 30220-46-3D, esters 67021-88-9 82425-34-1 **82425-35-2**
82438-00-4 82438-02-6 82468-50-6
RL: BIOL (Biological study)
(from Euphorbia kamerunica)
IT 30220-45-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

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=> d ibib abs hitstr ind 4
      3 ANSWERS ARE AVAILABLE.  SPECIFIED ANSWER NUMBER EXCEEDS ANSWER SET SIZE
The answer numbers requested are not in the answer set.
ENTER ANSWER NUMBER OR RANGE (1):end
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=> d ibib abs hitstr 1

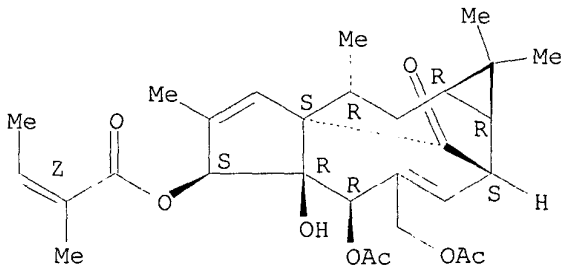
L17 ANSWER 1 OF 9 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1998:671897 HCAPLUS
DOCUMENT NUMBER: 130:35626
TITLE: Ingenane and lathyrane diterpenes from the latex of Euphorbia acrurensis
AUTHOR(S): Marco, J. Alberto; Sanz-Cervera, Juan F.; Ropero, F. Javier; Checa, Javier; Fraga, B. Manuel
CORPORATE SOURCE: Departamento de Quimica Organica, Universidad de Valencia, Valencia, E-46100, Spain
SOURCE: Phytochemistry (1998), 49(4), 1095-1099
CODEN: PYTCAS; ISSN: 0031-9422
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The latex of Euphorbia acrurensis yielded, in addn. to the widespread triterpenes euphol and euphorbol as the major components, two ingenol esters and nine lathyrane derivs. as minor components. All the lathyrane diterpenes were esters of ingol, and five of them were new. The structures were established with the aid of spectroscopic methods.

IT **88262-86-6 121570-35-2**
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)
(from latex of Euphorbia acrurensis)

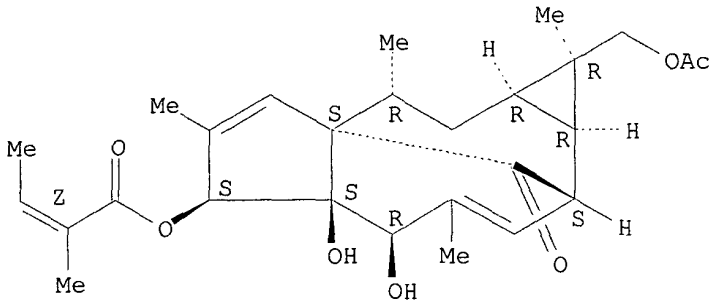
RN 88262-86-6 HCAPLUS
CN 2-Butenoic acid, 2-methyl-, (1aR,2S,5R,5aR,6S,8aS,9R,10aR)-5-(acetyloxy)-4-[(acetyloxy)methyl]-1a,2,5,5a,6,9,10,10a-octahydro-5a-hydroxy-1,1,7,9-tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



RN 121570-35-2 HCAPLUS
CN 2-Butenoic acid, 2-methyl-, (1R,1aR,2S,5R,5aS,6S,8aS,9R,10aR)-1-[(acetyloxy)methyl]-1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-1,4,7,9-tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d ind

L17 ANSWER 1 OF 9 HCAPLUS COPYRIGHT 2002 ACS
CC 11-1 (Plant Biochemistry)
Section cross-reference(s): 30
ST ingenane lathyrane diterpene Euphorbia
IT Diterpenes
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(from latex of Euphorbia acrurensis)
IT Euphorbia acrurensis
(ingenane and lathyrane diterpenes from latex of Euphorbia acrurensis)
IT Molecular structure, natural product
(of ingenol esters from Euphorbia acrurensis)
IT 514-47-6, Euphol 566-14-3, Euphorbol 58749-62-5 **88262-86-6**
89984-06-5 92910-93-5 92998-77-1 **121570-35-2**
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)
(from latex of Euphorbia acrurensis)
IT 216752-71-5P 216752-72-6P 216752-73-7P 216752-74-8P 216752-75-9P
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(from latex of Euphorbia acrurensis)

=> d ibib abs hitstr ind 2-9

L17 ANSWER 2 OF 9 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1998:348270 HCAPLUS
DOCUMENT NUMBER: 129:109225
TITLE: Diterpenes from Euphorbia paralias
AUTHOR(S): Jakupovic, J.; Morgenstern, T.; Marco, J. A.; Berendsohn, W.
CORPORATE SOURCE: Institute for Organic Chemistry, Technical University of Berlin, Berlin, D-10623, Germany
SOURCE: Phytochemistry (1998), 47(8), 1611-1619
CODEN: PYTCAS; ISSN: 0031-9422
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

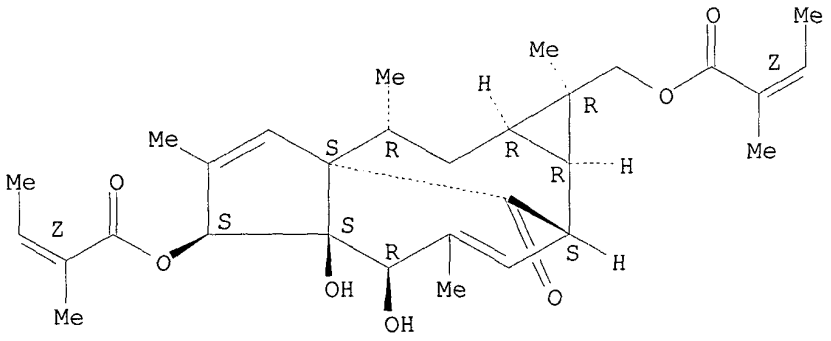
AB Chem. investigation of Euphorbia paralias from Spain afforded 13 diterpenes of different structural types, including one with a novel skeleton.

IT **210046-66-5P 210047-56-6P**
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); PROC (Process)
(isolation and characterization of diterpenes from Euphorbia paralias)

RN 210046-66-5 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, (1R,1aR,2S,5R,5aS,6S,8aS,9R,10aR)-1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-1,4,7,9-tetramethyl-1-[[[(2Z)-2-methyl-1-oxo-2-butenyl]oxy]methyl]-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, (2Z)-rel- (9CI) (CA INDEX NAME)

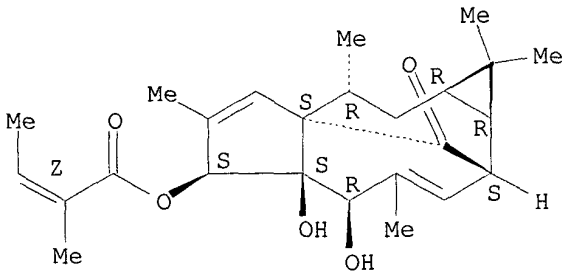
Relative stereochemistry.
Double bond geometry as shown.



RN 210047-56-6 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, (1aR,2S,5R,5aS,6S,8aS,9R,10aR)-1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-1,1,4,7,9-pentamethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, (2Z)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



CC 30-20 (Terpenes and Terpenoids)
Section cross-reference(s): 11

ST diterpene isolation Euphorbia paralias mol structure

IT Euphorbia paralias
(isolation and characterization of diterpenes from Euphorbia paralias)

IT Diterpenes

RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); PROC (Process)
(isolation and characterization of diterpenes from Euphorbia paralias)

IT Molecular structure, natural product
(of diterpenes)

IT 205870-73-1P 205870-75-3P 210046-57-4P 210046-58-5P 210046-59-6P 210046-60-9P 210046-61-0P 210046-62-1P 210046-63-2P 210046-64-3P 210046-65-4P **210046-66-5P 210047-56-6P**
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); PROC (Process)
(isolation and characterization of diterpenes from Euphorbia paralias)

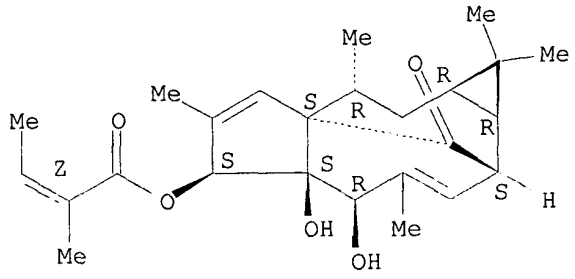
L17 ANSWER 3 OF 9 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1998:348268 HCAPLUS
DOCUMENT NUMBER: 129:120130
TITLE: Diterpenes from Euphorbia segetalis
AUTHOR(S): Jakupovic, J.; Jeske, F.; Morgenstern, T.; Tsichritzis, F.; Marco, J. A.; Berendsohn, W.
CORPORATE SOURCE: Institute for Organic Chemistry, Technical University of Berlin, Berlin, D-10623, Germany
SOURCE: Phytochemistry (1998), 47(8), 1583-1600
CODEN: PYTCAS; ISSN: 0031-9422
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Numerous new diterpenes including several with new skeletons have been obtained from Euphorbia segetalis.

IT **75567-38-3P 82425-35-2P 210158-15-9P 210158-16-0P 210158-17-1P**
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); PROC (Process)
(isolation and characterization of diterpenes from Euphorbia segetalis)

RN 75567-38-3 HCAPLUS
CN 2-Butenoic acid, 2-methyl-, (1aR,2S,5R,5aS,6S,8aS,9R,10aR)-1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-1,1,4,7,9-pentamethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, (2Z)- (9CI) (CA INDEX NAME)

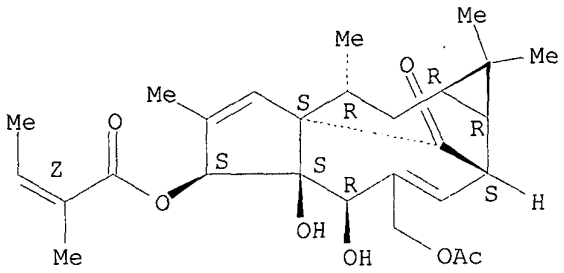
Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.



RN 82425-35-2 HCAPLUS

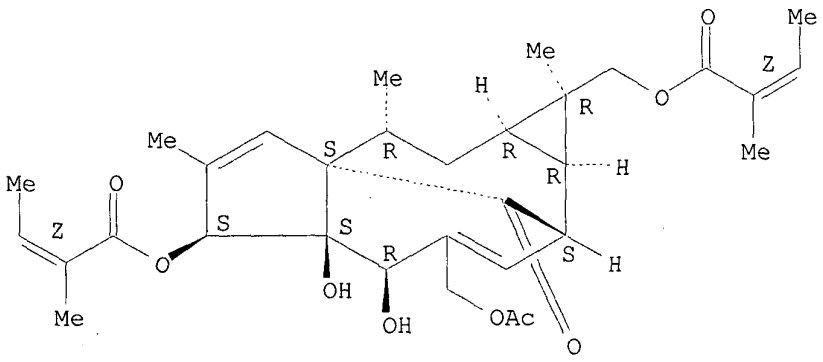
CN 2-Butenoic acid, 2-methyl-, (1aR,2S,5R,5aS,6S,8aS,9R,10aR)-4-[(acetyloxy)methyl]-1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-1,1,7,9-tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



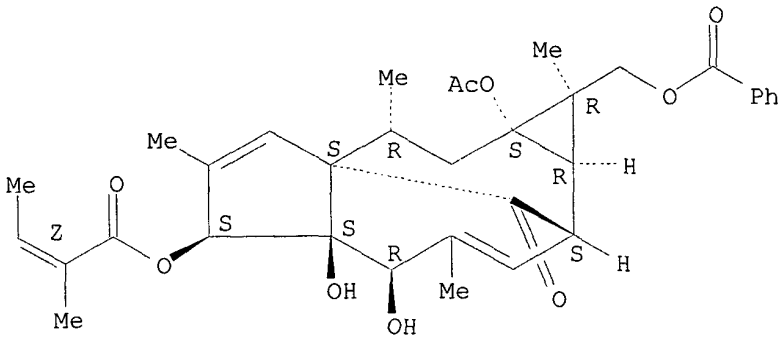
RN 210158-15-9 HCAPLUS
CN 2-Butenoic acid, 2-methyl-, (1R,1aR,2S,5R,5aS,6S,8aS,9R,10aR)-4-[(acetyloxy)methyl]-1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-1,7,9-trimethyl-1-[[[(2Z)-2-methyl-1-oxo-2-butenyl]oxy]methyl]-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



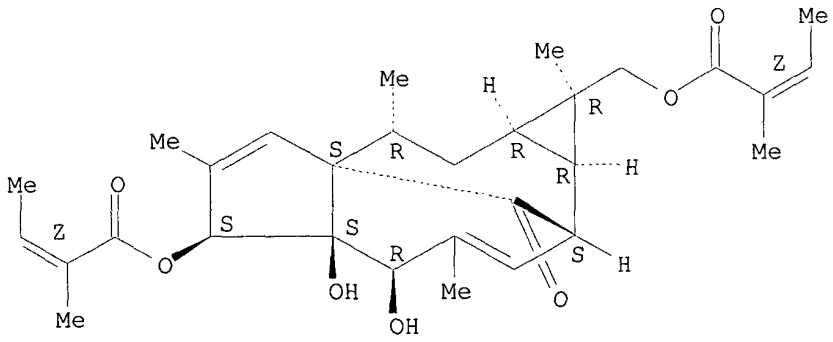
RN 210158-16-0 HCAPLUS
CN 2-Butenoic acid, 2-methyl-, (1R,1aR,2S,5R,5aS,6S,8aS,9R,10aS)-10a-(acetyloxy)-1-[(benzoyloxy)methyl]-1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-1,4,7,9-tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cycloprop a[e]cyclodecen-6-yl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 210158-17-1 HCAPLUS
CN 2-Butenoic acid, 2-methyl-, (1R,1aR,2S,5R,5aS,6S,8aS,9R,10aR)-
1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-1,4,7,9-tetramethyl-1-
[[[(2Z)-2-methyl-1-oxo-2-butenyl]oxy]methyl]-11-oxo-1H-2,8a-
methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, (2Z)- (9CI) (CA
INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

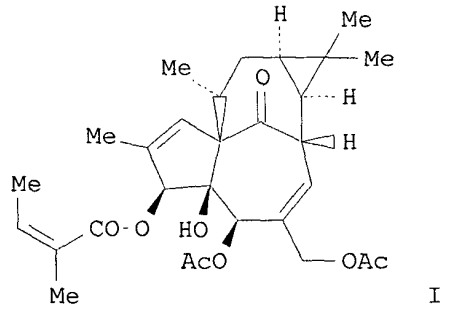


CC 11-1 (Plant Biochemistry)
Section cross-reference(s): 30
ST diterpene isolation Euphorbia segetalis
IT New natural products
(diterpenes from Euphorbia segetalis)
IT Euphorbia segetalis
(isolation and characterization of diterpenes from Euphorbia segetalis)
IT Diterpenes
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); PROC (Process)
(isolation and characterization of diterpenes from Euphorbia segetalis)
IT Molecular structure, natural product
(of diterpenes from Euphorbia segetalis)
IT 54706-99-9P 64280-37-1P **75567-38-3P 82425-35-2P**
129134-90-3P 174974-43-7P, Terracinolide A 174974-44-8P, Terracinolide B 190382-22-0P, Terracinolide C 190382-26-4P, Terracinolide E
210157-98-5P 210157-99-6P 210158-00-2P 210158-01-3P 210158-02-4P
210158-03-5P 210158-04-6P 210158-05-7P 210158-06-8P 210158-07-9P
210158-08-0P 210158-09-1P 210158-10-4P 210158-11-5P 210158-12-6P

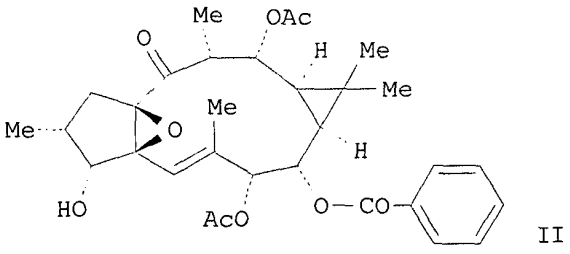
210158-13-7P 210158-14-8P **210158-15-9P 210158-16-0P**
210158-17-1P 210164-78-6P 210173-98-1P, Terracinolide H
210173-99-2P, Terracinolide I 210174-00-8P, 13.alpha.-Hydroxyterracinolide B 210174-01-9P, 13.alpha.-Hydroxyterracinolide I
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); PROC (Process)
(isolation and characterization of diterpenes from Euphorbia segetalis)

IT 210158-18-2P 210158-19-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(isolation and characterization of diterpenes from Euphorbia segetalis)

L17 ANSWER 4 OF 9 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1997:380090 HCAPLUS
DOCUMENT NUMBER: 127:119554
TITLE: Ingenane and lathyrane diterpenes from the latex of Euphorbia canariensis
AUTHOR(S): Marco, J. Alberto; Sanz-Cervera, Juan F.; Yuste, Alberto
CORPORATE SOURCE: Dep. Quimica Organica, Univ. Valencia, Burjassot, E-46100, Spain
SOURCE: Phytochemistry (1997), 45(3), 563-570
CODEN: PYTCAS; ISSN: 0031-9422
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I



II

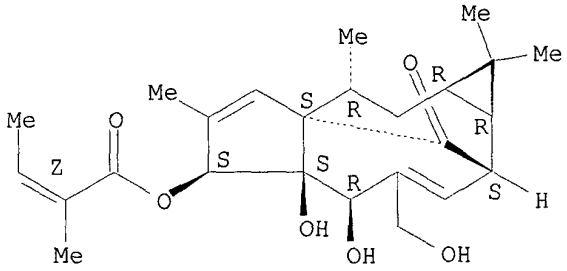
AB The latex of Euphorbia canariensis yielded, in addn. to five known ingenol esters, the ingenane derivs. ingenol 3-angelate 5,20-diacetate (I) and 5-deoxyingenol 3-angelate 20-acetate, and the lathyrane derivs. 2,3-diepiingol 7,12-diacetate 8-benzoate (II), 2,3-diepiingol 7,12-diacetate 8-isobutyrate and 2-epiingol 3,7,12-triacetate 8-benzoate.

The structures were established with the aid of spectroscopic methods, mainly NMR, and mol. mechanics calcns. They were also supported by the results of some chem. transformations.

IT **75567-37-2P 82425-35-2P 83966-48-7P 83983-93-1P 88262-75-3P 88262-86-6P 192825-63-1P 192825-64-2P**
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(ingenane and lathyrane diterpenes from the latex of Euphorbia canariensis)

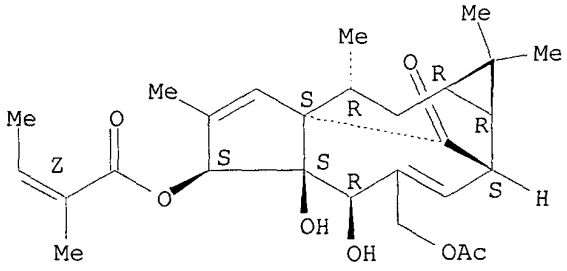
RN 75567-37-2 HCAPLUS
CN 2-Butenoic acid, 2-methyl-, (1aR,2S,5R,5aS,6S,8aS,9R,10aR)-1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-4-(hydroxymethyl)-1,1,7,9-tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



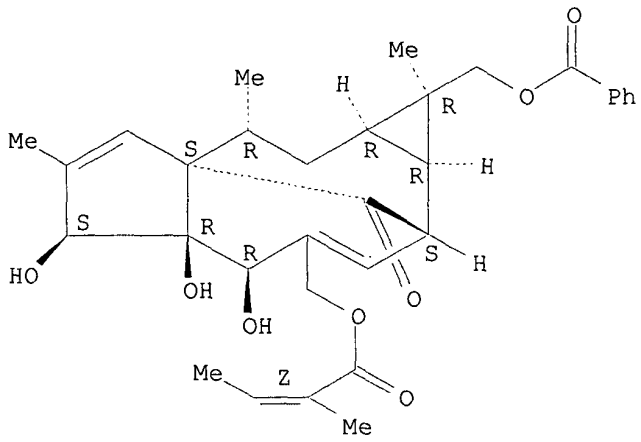
RN 82425-35-2 HCAPLUS
CN 2-Butenoic acid, 2-methyl-, (1aR,2S,5R,5aS,6S,8aS,9R,10aR)-4-[(acetyloxy)methyl]-1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-1,1,7,9-tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



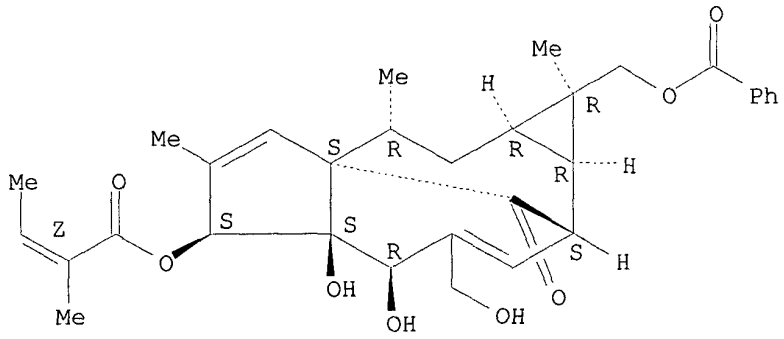
RN 83966-48-7 HCAPLUS
CN 2-Butenoic acid, 2-methyl-, [1-[(benzoyloxy)methyl]-1a,2,5,5a,6,9,10,10a-octahydro-5,5a,6-trihydroxy-1,7,9-trimethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-4-yl]methyl ester, [1R-[1.alpha.,1a.beta.,2.alpha.,4(Z),5.alpha.,5a.alpha.,6.alpha.,8a.beta.,9.beta.,10a.beta.]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.



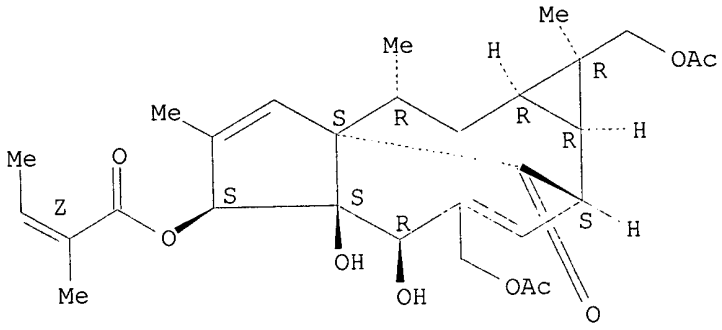
RN 83983-93-1 HCAPLUS
CN 2-Butenoic acid, 2-methyl-, (1R,1aR,2S,5R,5aS,6S,8aS,9R,10aR)-1-[(benzoyloxy)methyl]-1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-4-(hydroxymethyl)-1,7,9-trimethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



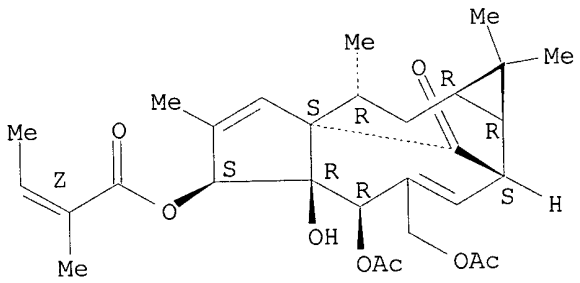
RN 88262-75-3 HCAPLUS
CN 2-Butenoic acid, 2-methyl-, 1,4-bis[(acetyloxy)methyl]-1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-1,7,9-trimethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, [1R-[1.alpha.,1a.beta.,2.alpha.,5.alpha.,5a.alpha.,6.alpha.(Z),8a.beta.,9.beta.,10a.beta.]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



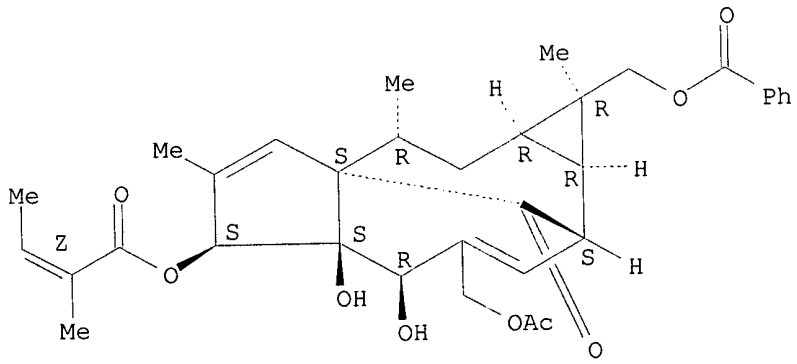
RN 88262-86-6 HCAPLUS
CN 2-Butenoic acid, 2-methyl-, (1aR,2S,5R,5aR,6S,8aS,9R,10aR)-5-(acetyloxy)-4-[(acetyloxy)methyl]-1a,2,5,5a,6,9,10,10a-octahydro-5a-hydroxy-1,1,7,9-tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



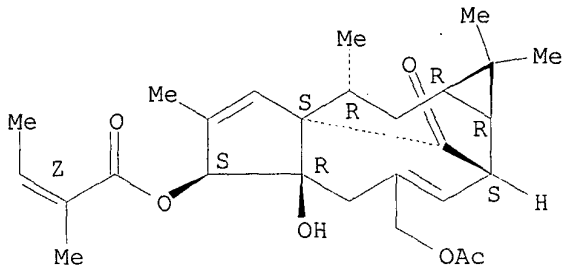
RN 192825-63-1 HCAPLUS
CN 2-Butenoic acid, 2-methyl-, (1R,1aR,2S,5R,5aS,6S,8aS,9R,10aR)-4-[(acetyloxy)methyl]-1-[(benzoyloxy)methyl]-1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-1,7,9-trimethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



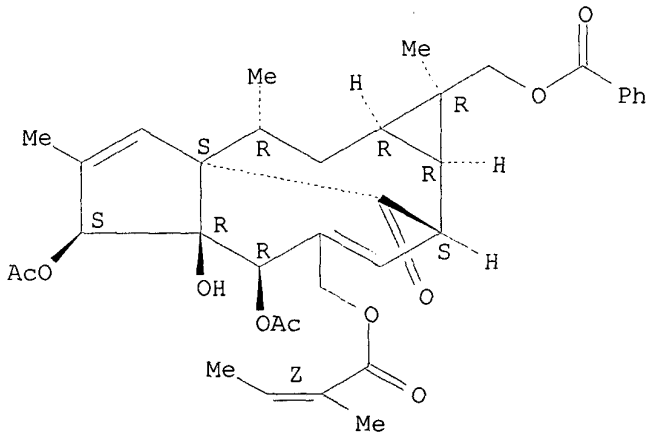
RN 192825-64-2 HCAPLUS
CN 2-Butenoic acid, 2-methyl-, 4-[(acetyloxy)methyl]-1a,2,5,5a,6,9,10,10a-octahydro-5a-hydroxy-1,1,7,9-tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, [1aR-[1a.alpha.,2.beta.,5a.beta.,6.beta.(Z),8a.alpha.,9.alpha.,10a.alpha.]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



IT **192825-66-4P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and properties of)
RN 192825-66-4 HCAPLUS
CN 2-Butenoic acid, 2-methyl-, 5,6-bis(acetyloxy)-[1-[(benzoyloxy)methyl]-1a,2,5,5a,6,9,10,10a-octahydro-5a-hydroxy-1,7,9-trimethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-4-yl]methyl ester, [1R-[1.alpha.,1a.beta.,2.alpha.,4(Z),5.alpha.,5a.alpha.,6.alpha.,8a.beta.,9.beta.,10a.beta.]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



CC 11-1 (Plant Biochemistry)
Section cross-reference(s): 30
ST ingenane lathyrane diterpene Euphorbia
IT Euphorbia canariensis
(ingenane and lathyrane diterpenes from the latex of Euphorbia canariensis)

IT Diterpenes
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(ingenane and lathyrane diterpenes from the latex of Euphorbia canariensis)

IT **75567-37-2P 82425-35-2P 83966-48-7P**
83983-93-1P 88262-75-3P 88262-86-6P
192045-51-5P **192825-63-1P 192825-64-2P** 192825-65-3P
192865-19-3P
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(ingenane and lathyrane diterpenes from the latex of Euphorbia canariensis)

IT **192825-66-4P** 192865-20-6P 192865-24-0P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and properties of)

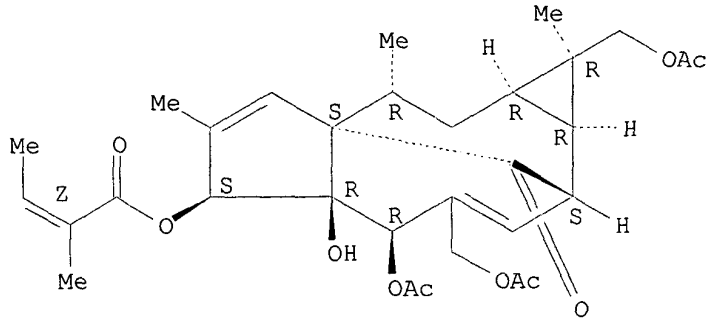
L17 ANSWER 5 OF 9 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1984:607619 HCAPLUS
DOCUMENT NUMBER: 101:207619
TITLE: Five ingol esters and a 17-hydroxyingenol ester from the latex of Euphorbia kamerunica. Assignment of esters using carbon-13 NMR methods
AUTHOR(S): Connolly, Joseph D.; Fakunle, Christopher O.; Rycroft, David S.
CORPORATE SOURCE: Dep. Chem., Univ. Glasgow, Glasgow, G12 8QQ, UK
SOURCE: Tetrahedron Letters (1984), 25(34), 3773-6
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The structures of 5 ingol esters and a 17-hydroxyingenol ester from the latex of E. kamerunica were detd. The 13C NMR spectra of these compds. have been assigned using 2D .delta.C/.beta.H correlations. The specific positions of attachment of esters have been assigned unambiguously using 13C NMR methods, including 2D long-range .delta.C/.delta.H correlations. The 5 ingol esters were 8-O-methylingol-3,12-diacetate-7-tiglate, 8-O-methylingol-3,12-diacetate-7-benzoate, ingol-3,8,12-triacetate-7-tiglate, ingol-3,8,12-triacetate-7-angelate, and 8-O-methylingol-3,12-diacetate-7-angelate.

IT **92998-75-9**
RL: BIOL (Biological study)
(from latex of Euphorbia kamerunica)

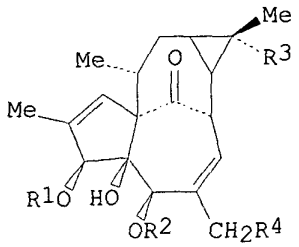
RN 92998-75-9 HCAPLUS
CN 2-Butenoic acid, 2-methyl-, 5-(acetyloxy)-1,4-bis[(acetyloxy)methyl]-1a,2,5,5a,6,9,10,10a-octahydro-5a-hydroxy-1,7,9-trimethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, [1R-[1.alpha.,1a.beta.,2.alpha.,5.alpha.,5a.alpha.,6.alpha.(Z),8a.beta.,9.beta.,10a.beta.]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



CC 11-1 (Plant Biochemistry)
ST ingol ester Euphorbia latex; hydoxyingenol ester Euphorbia latex
IT Euphorbia kamerunica
(ingol esters from latex of)
IT Latex
(ingol esters from, Euphorbia kamerunica)
IT 89984-05-4 89984-06-5 90027-10-4 92910-93-5 **92998-75-9**
92998-77-1
RL: BIOL (Biological study)
(from latex of Euphorbia kamerunica)

L17 ANSWER 6 OF 9 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1984:20456 HCAPLUS
DOCUMENT NUMBER: 100:20456
TITLE: The dermatitis-producing constituents of Euphorbia hermentiana latex
AUTHOR(S): Lin, Lee Juian; Marshall, Gary T.; Kinghorn, A. Douglas
CORPORATE SOURCE: Coll. Pharm., Univ. Illinois, Chicago, IL, 60612, USA
SOURCE: Journal of Natural Products (1983), 46(5), 723-31
CODEN: JNPRDF; ISSN: 0163-3864
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I, R^1=Pr(CH:CH)$_3$CO, R^2=H, R^3=CH_2O_2CCMe:CHMe, R^4=OH

II, R^1=MeCH:$CMeCO_2$, R^2=Ac, R^3=CH_2OAc, R^4=OAc

III, R^1=MeCH:$CMeCO_2$, R^2=H, R^3=CH_2OAc, R^4=OAc

IV, R^1=MeCH:$CMeCO_2$, R^2=H, R^3=Me, R^4=OAc

V, R^1=MeCH:$CMeCO_2$, R^2=R^4=H, R^3=CH_2OAc

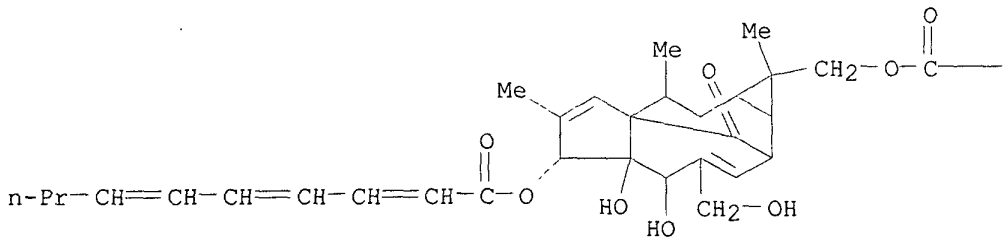
AB Five ingenane derivs. 3-O-n-(deca-2,4,6-trienoyl)-16-O-[(Z)-2-methyl-2-butenoyl]-16-hydroxyingenol(I), 3-O-[(Z)-2-methyl-2-butenoyl]-5,16,20-O-triacetyl-16-hydroxyingenol(II), 3-O-[(Z)-2-methyl-2-butenoyl]-16,20-O-diacetyl-16-hydroxyingenol(III), 3-O-[(Z)-2-methyl-2-butenoyl]-20-O-acetylingenol(IV), and 3-O-[(Z)-2-methyl-2-butenoyl]-16-O-acetyl-20-deoxy-16-hydroxyingenol(V) were isolated with a new procedure that uses droplet counter-current chromatog., from a dermatitis-producing fraction of the latex of E. hermentiana. The structures of II, III, and V were established by the interpretation of their spectroscopic data and those of their hydrolytic and acetylated derivs.

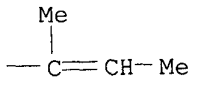
IT **52557-27-4 82425-35-2 88262-74-2**
88262-75-3 88262-77-5
RL: BIOL (Biological study)
(of Euphorbia hermentiana latex, dermatitis-producing)

RN 52557-27-4 HCAPLUS

CN 2,4,6-Decatrienoic acid, (1S,1aR,2S,5R,5aR,6S,8aS,9R,10aR)-1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-4-(hydroxymethyl)-1,7,9-trimethyl-1-[[[(2Z)-2-methyl-1-oxo-2-butenyl]oxy]methyl]-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester (9CI) (CA INDEX NAME)

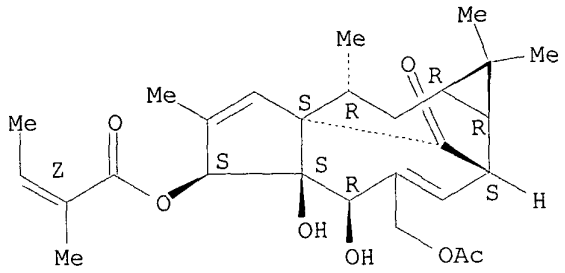
PAGE 1-A





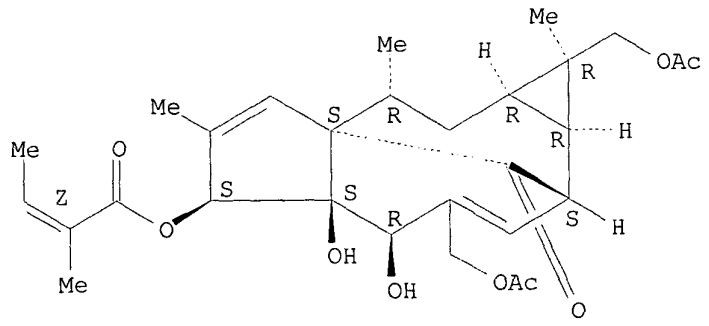
RN 82425-35-2 HCAPLUS
CN 2-Butenoic acid, 2-methyl-, (1aR,2S,5R,5aS,6S,8aS,9R,10aR)-4-[(acetyloxy)methyl]-1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-1,1,7,9-tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



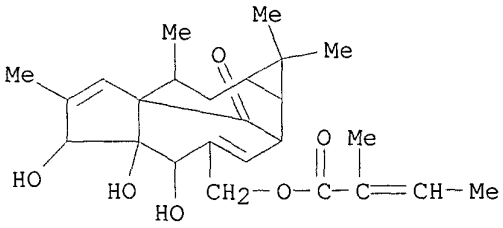
RN 88262-74-2 HCAPLUS
RN 88262-75-3 HCAPLUS
CN 2-Butenoic acid, 2-methyl-, 1,4-bis[(acetyloxy)methyl]-1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-1,7,9-trimethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, [1R-[1.alpha.,1a.beta.,2.alpha.,5.alpha.,5a.alpha.,6.alpha.(Z),8a.beta.,9.beta.,10a.beta.]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



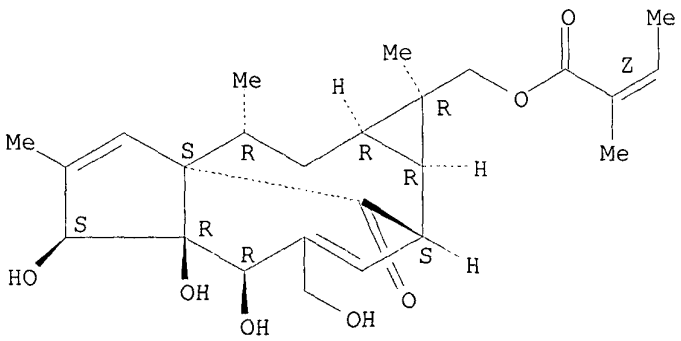
RN 88262-77-5 HCAPLUS
IT **83966-49-8P 88262-78-6P 88262-79-7P**
88262-81-1P 88262-82-2P 88262-84-4P
88262-85-5P 88262-86-6P 88262-88-8P
88262-90-2P 88262-91-3P 88262-92-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 83966-49-8 HCAPLUS
CN 2-Butenoic acid, 2-methyl-, (1a,2,5,5a,6,9,10,10a-octahydro-5,5a,6-trihydroxy-1,1,7,9-tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-4-yl)methyl ester, [1aR-[1a.alpha.,2.beta.,4(Z),5.beta.,5a.beta.,6.beta.,8a.alpha.,9.alpha.,10a.alpha.]]- (9CI) (CA INDEX NAME)



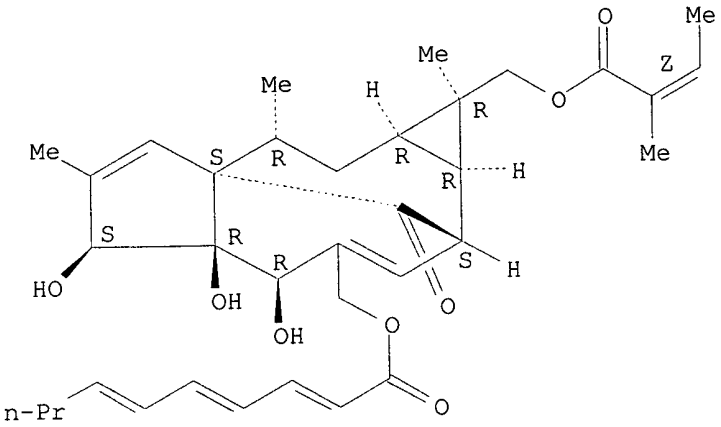
RN 88262-78-6 HCAPLUS
CN 2-Butenoic acid, 2-methyl-, [1a,2,5,5a,6,9,10,10a-octahydro-5,5a,6-trihydroxy-4-(hydroxymethyl)-1,7,9-trimethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-1-yl]methyl ester, [1R-[1.alpha.(Z),1a.beta.,2.alpha.,5.alpha.,5a.alpha.,6.alpha.,8a.beta.,9.beta.,10a.beta.]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



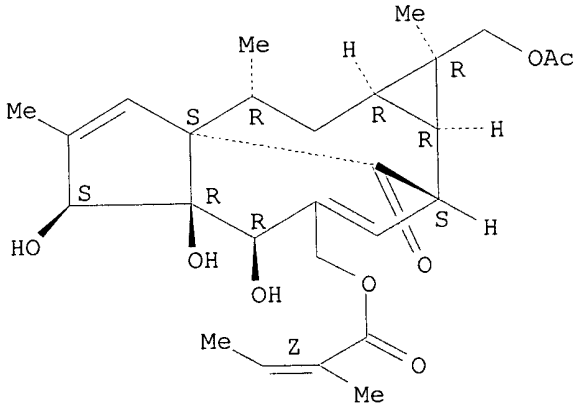
RN 88262-79-7 HCAPLUS
CN 2,4,6-Decatrienoic acid, [1a,2,5,5a,6,9,10,10a-octahydro-5,5a,6-trihydroxy-1,7,9-trimethyl-1-[[(2-methyl-1-oxo-2-butenyl)oxy]methyl]-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-4-yl]methyl ester, [1R-[1.alpha.(Z),1a.beta.,2.alpha.,5.alpha.,5a.alpha.,6.alpha.,8a.beta.,9.beta.,10a.beta.]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as described by E or Z.



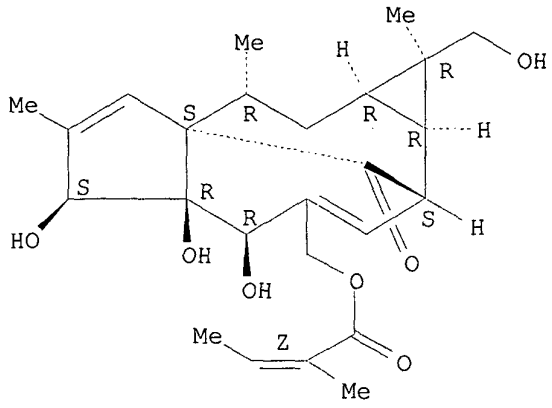
RN 88262-81-1 HCAPLUS
CN 2-Butenoic acid, 2-methyl-, [1-[(acetyloxy)methyl]-1a,2,5,5a,6,9,10,10a-octahydro-5,5a,6-trihydroxy-1,7,9-trimethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-4-yl]methyl ester, [1R-[1.alpha.,1a.beta.,2.alpha.,4(Z),5.alpha.,5a.alpha.,6.alpha.,8a.beta.,9.beta.,10a.beta.]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



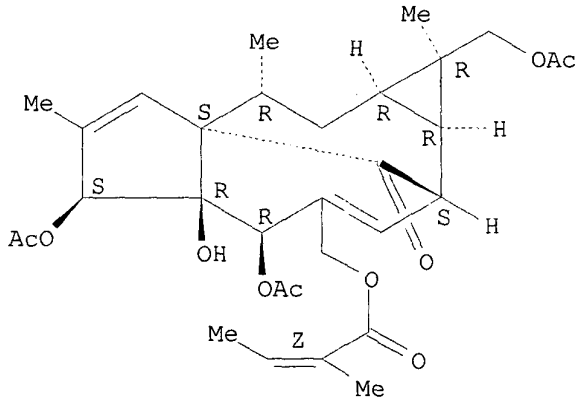
RN 88262-82-2 HCAPLUS
CN 2-Butenoic acid, 2-methyl-, [1a,2,5,5a,6,9,10,10a-octahydro-5,5a,6-trihydroxy-1-(hydroxymethyl)-1,7,9-trimethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-4-yl]methyl ester, [1R-[1.alpha.,1a.beta.,2.alpha.,4(Z),5.alpha.,5a.alpha.,6.alpha.,8a.beta.,9.beta.,10a.beta.]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



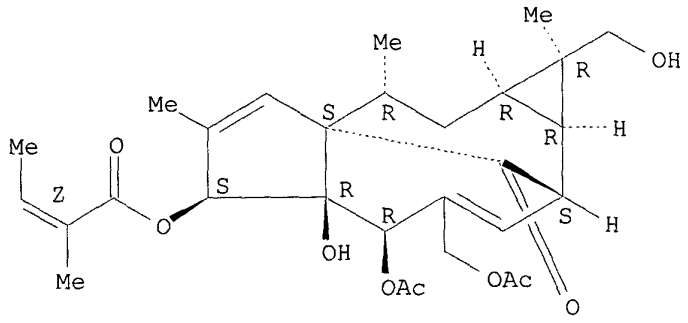
RN 88262-84-4 HCAPLUS
CN 2-Butenoic acid, 2-methyl-, [5,6-bis(acetyloxy)-1-[(acetyloxy)methyl]-1a,2,5,5a,6,9,10,10a-octahydro-5a-hydroxy-1,7,9-trimethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-4-yl]methyl ester, [1R-[1.alpha.,1a.beta.,2.alpha.,4(Z),5.alpha.,5a.alpha.,6.alpha.,8a.beta.,9.beta.,10a.beta.]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



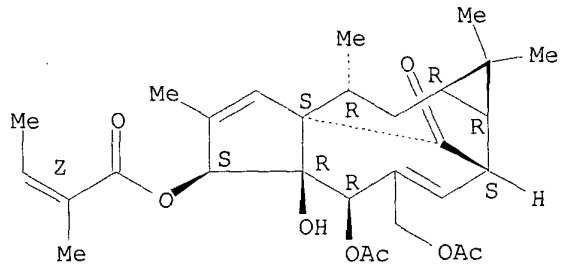
RN 88262-85-5 HCAPLUS
CN 2-Butenoic acid, 2-methyl-, 5-(acetyloxy)-4-[(acetyloxy)methyl]-1a,2,5,5a,6,9,10,10a-octahydro-5a-hydroxy-1-(hydroxymethyl)-1,7,9-trimethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, [1R-[1.alpha.,1a.beta.,2.alpha.,5.alpha.,5a.alpha.,6.alpha.(Z),8a.beta.,9.beta.,10a.beta.]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

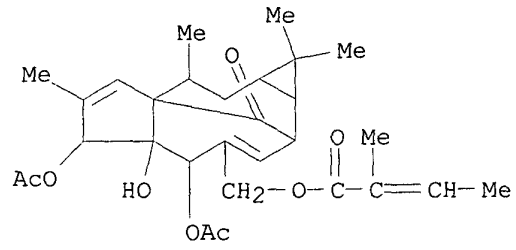


RN 88262-86-6 HCAPLUS
CN 2-Butenoic acid, 2-methyl-, (1aR,2S,5R,5aR,6S,8aS,9R,10aR)-5-(acetyloxy)-4-[(acetyloxy)methyl]-1a,2,5,5a,6,9,10,10a-octahydro-5a-hydroxy-1,1,7,9-tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.

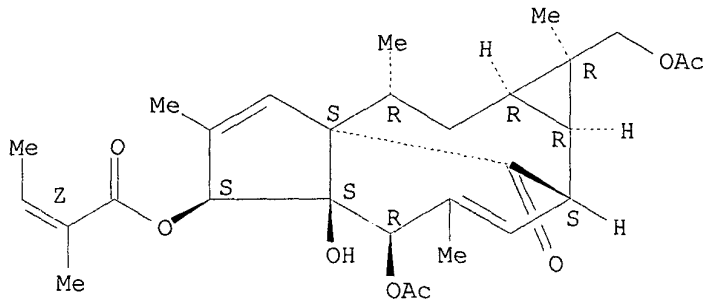


RN 88262-88-8 HCAPLUS
CN 2-Butenoic acid, 2-methyl-, [5,6-bis(acetyloxy)-1a,2,5,5a,6,9,10,10a-octahydro-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-4-yl]methyl ester, [1aR-[1a.alpha.,2.beta.,4(Z),5.beta.,5a.beta.,6.beta.,8a.alpha.,9.alpha.,10a.alpha.]]- (9CI) (CA INDEX NAME)



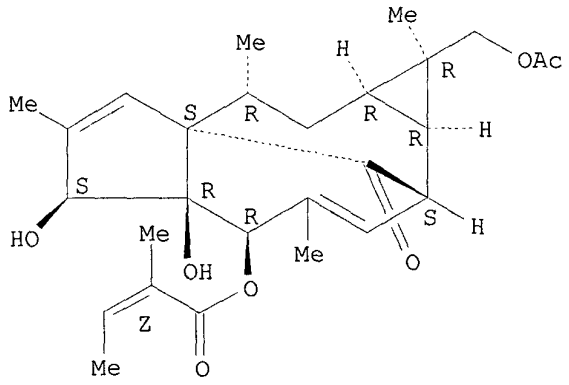
RN 88262-90-2 HCAPLUS
CN 2-Butenoic acid, 2-methyl-, 5-(acetyloxy)-1-[(acetyloxy)methyl]-1a,2,5,5a,6,9,10,10a-octahydro-5a-hydroxy-1,4,7,9-tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, [1R-[1.alpha.,1a.beta.,2.alpha.,5.alpha.,5a.alpha.,6.alpha.(Z),8a.beta.,9.beta.,10a.beta.]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



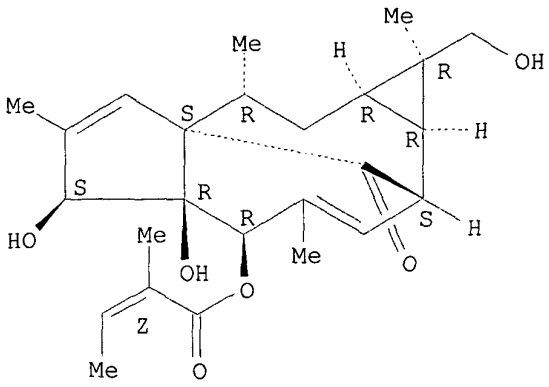
RN 88262-91-3 HCAPLUS
CN 2-Butenoic acid, 2-methyl-, 1-[(acetyloxy)methyl]-1a,2,5,5a,6,9,10,10a-octahydro-5a,6-dihydroxy-1,4,7,9-tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-5-yl ester, [1R-[1.alpha.,1a.beta.,2.alpha.,5.alpha.(Z),5a.alpha.,6.alpha.,8a.beta.,9.beta.,10a.beta.]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



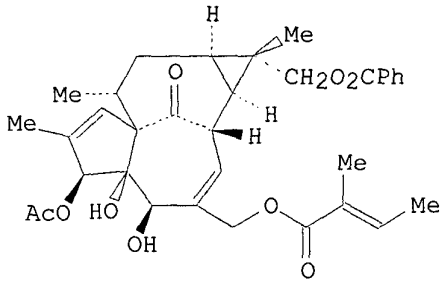
RN 88262-92-4 HCAPLUS
CN 2-Butenoic acid, 2-methyl-, 1a,2,5,5a,6,9,10,10a-octahydro-5a,6-dihydroxy-1-(hydroxymethyl)-1,4,7,9-tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-5-yl ester, [1R-[1.alpha.,1a.beta.,2.alpha.,5.alpha.(Z),5a.alpha.,6.alpha.,8a.beta.,9.beta.,10a.beta.]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



CC 11-1 (Plant Biochemistry)
Section cross-reference(s): 1, 30, 63
ST Euphorbia ingenane deriv; dermatitis Euphorbia ingenol deriv; diterpene Euphorbia ingenol deriv
IT Dermatitis
(from ingenane derivs. of Euphorbia hermentiana latex)
IT Euphorbia trigona
(ingenane derivs. of, dermatitis-producing)
IT Diterpenes and Diterpenoids
RL: BIOL (Biological study)
(of Euphorbia hermentiana latex, dermatitis-producing)
IT 83036-62-8
RL: BIOL (Biological study)
(acyl rearrangement of with acium hydroxide)
IT **52557-27-4 82425-35-2 88262-74-2**
88262-75-3 88262-77-5
RL: BIOL (Biological study)
(of Euphorbia hermentiana latex, dermatitis-producing)
IT 30220-45-2P 52557-30-9P **83966-49-8P 88262-78-6P**
88262-79-7P 88262-81-1P 88262-82-2P
88262-83-3P **88262-84-4P 88262-85-5P**
88262-86-6P 88262-88-8P 88262-90-2P
88262-91-3P 88262-92-4P 88262-93-5P 88262-95-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

L17 ANSWER 7 OF 9 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1983:122775 HCAPLUS
DOCUMENT NUMBER: 98:122775
TITLE: Three new ingenane derivatives from the latex of Euphorbia canariensis L
AUTHOR(S): Lin, Lee Juian; Kinghorn, A. Douglas
CORPORATE SOURCE: Coll. Pharm., Univ. Illinois, Chicago, IL, 60612, USA
SOURCE: Journal of Agricultural and Food Chemistry (1983), 31(2), 396-400
CODEN: JAFCAU; ISSN: 0021-8561
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



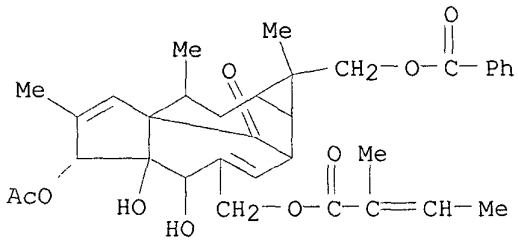
I

AB Three new ingenane esters, 3-O-acetyl-16-O-benzoyl-20-O-[(Z)-2-methyl-2-butenoyl]-16-hydroxyingenol (I), 3-O-[(Z)-2-methyl-2-butenoyl]-16-O-benzoyl-16-hydroxyingenol, and 3-O-acetyl-20-O-[(Z)-2-methyl-2-butenoyl]ingenol, were isolated from the latex of E. canariensis by using droplet countercurrent chromatog. The structures of these compds. were established through the interpretation of spectroscopic data. The compds. are known skin irritants.

IT **83966-45-4 83966-46-5 83983-93-1**
RL: BIOL (Biological study)
(of Euphorbia canariensis latex)

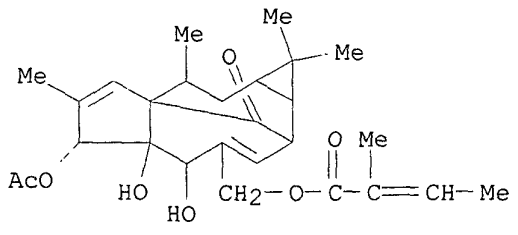
RN 83966-45-4 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, [6-(acetyloxy)-1-[(benzoyloxy)methyl]-1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-1,7,9-trimethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-4-yl]methyl ester, [1S-[1.alpha.,1a.alpha.,2.beta.,4(Z),5.beta.,5a.beta.,6.beta.,8a.alpha.,9.alpha.,10a.alpha.]]- (9CI) (CA INDEX NAME)



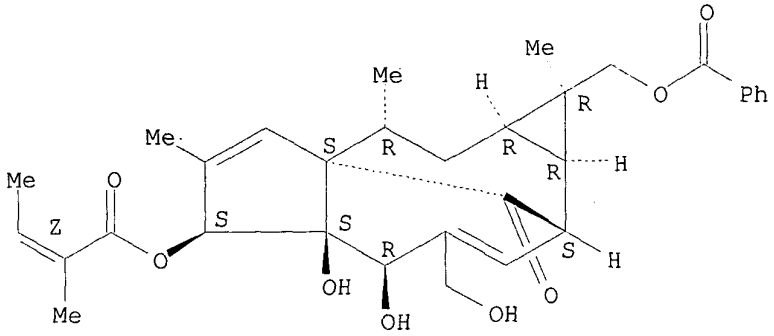
RN 83966-46-5 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, [6-(acetyloxy)-1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-1,1,7,9-tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-4-yl]methyl ester, [1aR-[1a.alpha.,2.beta.,4(Z),5.beta.,5a.beta.,6.beta.,8a.alpha.,9.alpha.,10a.alpha.]]- (9CI) (CA INDEX NAME)



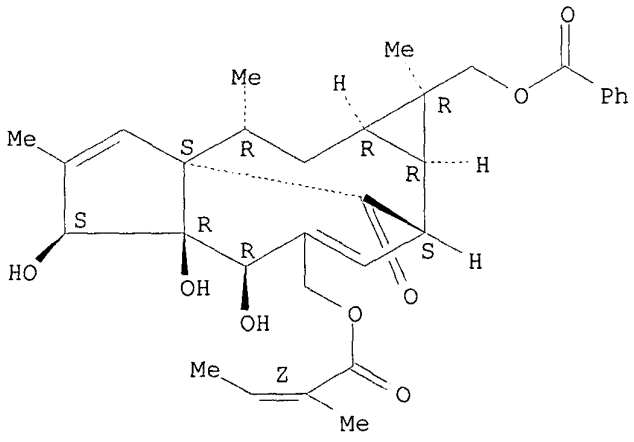
RN 83983-93-1 HCAPLUS
CN 2-Butenoic acid, 2-methyl-, (1R,1aR,2S,5R,5aS,6S,8aS,9R,10aR)-1-[(benzoyloxy)methyl]-1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-4-(hydroxymethyl)-1,7,9-trimethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



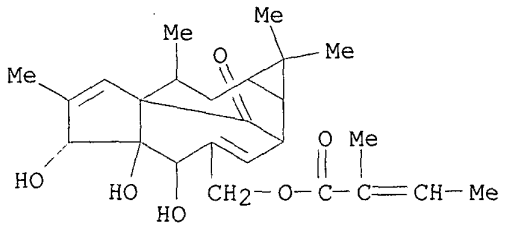
IT **83966-48-7P 83966-49-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 83966-48-7 HCAPLUS
CN 2-Butenoic acid, 2-methyl-, [1-[(benzoyloxy)methyl]-1a,2,5,5a,6,9,10,10a-octahydro-5,5a,6-trihydroxy-1,7,9-trimethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-4-yl]methyl ester, [1R-[1.alpha.,1a.beta.,2.alpha.,4(Z),5.alpha.,5a.alpha.,6.alpha.,8a.beta.,9.beta.,10a.beta.]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.



RN 83966-49-8 HCAPLUS
CN 2-Butenoic acid, 2-methyl-, (1a,2,5,5a,6,9,10,10a-octahydro-5,5a,6-trihydroxy-1,1,7,9-tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-4-yl)methyl ester,

[1aR-[1a.alpha.,2.beta.,4(Z),5.beta.,5a.beta.,6.beta.,8a.alpha.,9.alpha.,10a.alpha.]]- (9CI) (CA INDEX NAME)

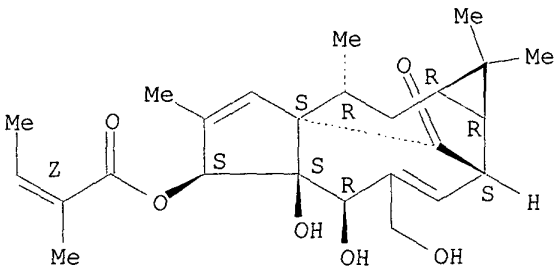


CC 11-1 (Plant Biochemistry)
ST Euphorbia diterpene ester ingenane; ingenane latex Euphorbia
IT Euphorbia canariensis
(diterpene esters of latex of)
IT Diterpenes and Diterpenoids
RL: BIOL (Biological study)
(esters, of Euphorbia canariensis)
IT **83966-45-4 83966-46-5 83983-93-1**
RL: BIOL (Biological study)
(of Euphorbia canariensis latex)
IT 30220-45-2P 52557-30-9P 83966-47-6P **83966-48-7P**
83966-49-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

L17 ANSWER 8 OF 9 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1980:617929 HCAPLUS
DOCUMENT NUMBER: 93:217929
TITLE: Constituents of Egyptian Euphorbiaceae. IX. Irritant and cytotoxic ingenane esters from Euphorbia paralias L
AUTHOR(S): Sayed, M. D.; Riszk, A.; Hammouda, F. M.; El-Missiry, M. M.; Williamson, E. M.; Evans, F. J.
CORPORATE SOURCE: Pharm. Sci. Lab., Natl. Res. Cent., Cairo, Egypt
SOURCE: Experientia (1980), 36(10), 1206-7
CODEN: EXPEAM; ISSN: 0014-4754
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The irritant and cytotoxic constituents of the latex of E. paralias were sepd. from the hydrocarbon fraction by solvent partition. Three new ingenane esters were identified from the toxic ether fraction. The major compd. was 3-angelyl-20-deoxyingenol and the 2 minor compds. were 3-hexanoyl-20-deoxyingenol and 3-angelylingenol. These compds. were of a similar potency to podophyllin in the inhibition of thymidine-3H uptake by TLX/5 mouse lymphoma cells. In addn., the compds. produced a persistent erythema of the mouse ear in sub-microgram doses.
IT **75567-37-2 75567-38-3**
RL: BIOL (Biological study)
(from Euphorbia paralias, cytotoxic and irritant activities of)
RN 75567-37-2 HCAPLUS
CN 2-Butenoic acid, 2-methyl-, (1aR,2S,5R,5aS,6S,8aS,9R,10aR)-1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-4-(hydroxymethyl)-1,1,7,9-tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, (2Z)- (9CI) (CA INDEX NAME)

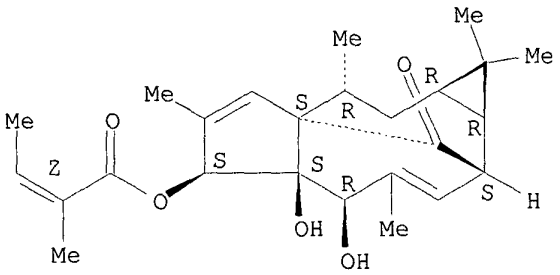
Absolute stereochemistry. Rotation (+).

Double bond geometry as shown.



RN 75567-38-3 HCAPLUS
CN 2-Butenoic acid, 2-methyl-, (1aR,2S,5R,5aS,6S,8aS,9R,10aR)-1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-1,1,4,7,9-pentamethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, (2Z)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.

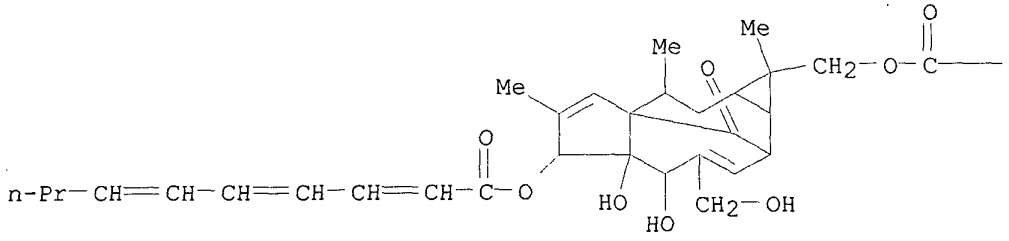


CC 11-1 (Plant Biochemistry)
Section cross-reference(s): 1
ST ingenane ester Euphorbia
IT Diterpenes and Diterpenoids
RL: BIOL (Biological study)
(from Euphorbia paralias, cytotoxic and irritant activities of)
IT Euphorbia paralias
(ingenane esters from, cytotoxic and irritant activity of)
IT Cytotoxic agents
(ingenane esters, from Euphorbia paralias)
IT **75567-37-2 75567-38-3** 75567-39-4
RL: BIOL (Biological study)
(from Euphorbia paralias, cytotoxic and irritant activities of)
IT 30220-46-3P 54706-99-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and acetylation of)
IT 30220-45-2P 54707-00-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

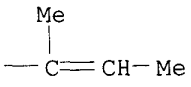
L17 ANSWER 9 OF 9 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1974:146346 HCAPLUS
DOCUMENT NUMBER: 80:146346
TITLE: New diterpenoid irritants from Euphorbia ingens
AUTHOR(S): Opferkuch, H. J.; Hecker, E.

CORPORATE SOURCE: Inst. Biochem., Dtsch. Krebsforschungszent., Heidelberg, Ger.
SOURCE: Tetrahedron Lett. (1974), (3), 261-4
CODEN: TELEAY
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB The irritants I, II, and III, and the non-irritants IV and the 3,7,12-triacetate-8-nicotinate of ingol, were isolated from the latex of Euphorbia ingens. On the mouse ear, III showed an irritant dose 50 of 0.02 .mu.g/ear and II a dose of 0.004 .mu./ear.
IT **52557-27-4**
RL: BOC (Biological occurrence); BIOL (Biological study); OCCU (Occurrence)
(of Euphorbia ingens)
RN 52557-27-4 HCAPLUS
CN 2,4,6-Decatrienoic acid, (1S,1aR,2S,5R,5aR,6S,8aS,9R,10aR)-1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-4-(hydroxymethyl)-1,7,9-trimethyl-1-[[[(2Z)-2-methyl-1-oxo-2-butenyl]oxy]methyl]-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



CC 30-20 (Terpenoids)
Section cross-reference(s): 11
ST Euphorbia terpenoid irritant
IT Skin, toxic chemical and physical damage
(for Euphorbia ingens diterpenoids)
IT Diterpenoids
RL: BOC (Biological occurrence); BIOL (Biological study); OCCU (Occurrence)
(of Euphorbia ingens)
IT Euphorbia ingens
(terpenoid irritants of)
IT 39071-33-5 51906-00-4 52557-26-3 **52557-27-4** 52557-28-5
RL: BOC (Biological occurrence); BIOL (Biological study); OCCU (Occurrence)
(of Euphorbia ingens)
IT 52557-29-6P 52557-30-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

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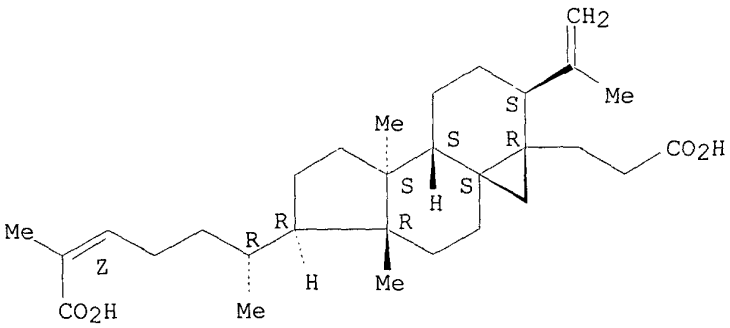
L22 ANSWER 1 OF 16 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2001:439629 HCAPLUS
DOCUMENT NUMBER: 136:256788
TITLE: Triterpenoid acids from Schisandra propinqua with cytotoxic effect on rat luteal cells and human decidual cells in vitro
AUTHOR(S): Chen, Y.-G.; Qin, G.-W.; Cao, L.; Leng, Y.; Xie, Y.-Y.
CORPORATE SOURCE: Department of Chemistry, Yunnan Normal University, Kunming, Yunnan, 650092, Peop. Rep. China
SOURCE: Fitoterapia (2001), 72(4), 435-437
CODEN: FTRPAE; ISSN: 0367-326X
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Three triterpenoid acids, nigranoic acid (1), manwuweizic acid (2), schisandronic acid (3), and other four compds. were isolated from the stems of Schisandra propinqua. Compds. 1 and 2 showed significant cytotoxic effect against human decidual cells and rat luteal cells in vitro.

IT **39111-07-4P**, Nigranoic acid **55511-14-3P**, Schisandronic acid
RL: **PAC (Pharmacological activity)**; PUR (Purification or recovery); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(triterpenoid acids from Schisandra propinqua with cytotoxic effect on rat luteal cells and human decidual cells in vitro)

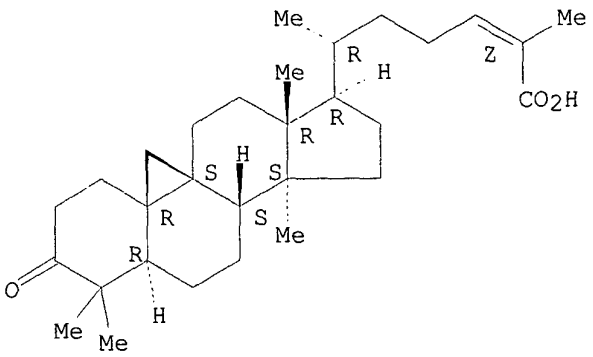
RN 39111-07-4 HCAPLUS
CN 1H-Cyclopenta[a]cyclopropa[e]naphthalene-3a(4H)-propanoic acid, 7-[(1R,4Z)-5-carboxy-1-methyl-4-hexenyl]decahydro-6a,9a-dimethyl-3-(1-methylethenyl)-, (3S,3aR,4aS,6aR,7R,9aS,9bS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 55511-14-3 HCAPLUS
CN 9,19-Cyclolanost-24-en-26-oic acid, 3-oxo-, (24Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 2 OF 16 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2000:456898 HCAPLUS
DOCUMENT NUMBER: 133:88533
TITLE: Compositions obtained from Mangifera indica L.
INVENTOR(S): Nunez Selles, Alberto Julio; Paez Betancourt, Eleuterio; Amaro Gonzalez, Daniel; Acosta Esquijarosa, Jhoany; Aguero Aguero, Juan; Capote Hernandez, Raul; Garciga Hernandez, Maria Rosa; Morales Lacarrere, Ivan Gaston; Garcia Pulpeiro, Oscar; Garrido Garrido, Gabino; Martinez Sanchez, Gregorio; Morales, Miguel
PATENT ASSIGNEE(S): Centro de Quimica Farmaceutica, Cuba
SOURCE: PCT Int. Appl., 34 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Spanish
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000038699	A1	20000706	WO 1999-CU7	19991229

W: AU, BR, CA, CN, ID, IN, JP, MX, RU, SD, UA, US, VN
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

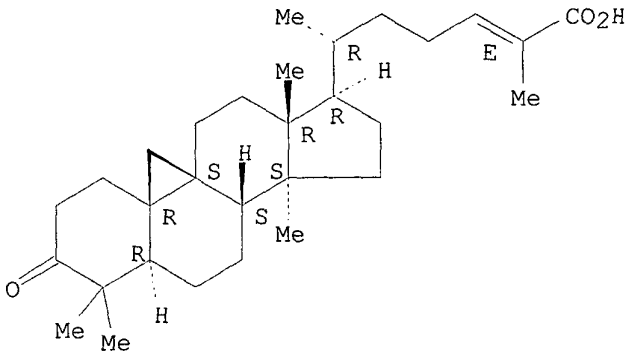
PRIORITY APPLN. INFO.: CU 1998-203 A 19981229

AB The present invention relates essentially to the pharmaceutical, food and cosmetic industries and in particular to the prepn. of formulations of active principles which are derived from bark of the plant Mangifera indica, among which are the polyphenols, the terpenoids, the steroids, the fatty acids and microelements which have antioxidant, anti-**inflammatory**, analgesic and antispasmodic properties, thereby conferring to said formulations high value as dietary supplements for the improvement of the quality of life of patients suffering from degenerative diseases, as well as for anti-aging treatment and for consumption by healthy persons.

IT **13878-90-5**, Mangiferonic acid
RL: BUU (Biological use, unclassified); FFD (Food or feed use); **THU (Therapeutic use)**; BIOL (Biological study); USES (Uses)
(compns. obtained from Mangifera indica for health food and drugs and cosmetics)
RN 13878-90-5 HCAPLUS

CN 9,19-Cyclolanost-24-en-26-oic acid, 3-oxo-, (24E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 3 OF 16 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1999:567080 HCAPLUS
DOCUMENT NUMBER: 131:317356
TITLE: Activity of triterpenoid glycosides from the root bark of Mussaenda macrophylla against two oral pathogens
AUTHOR(S): Kim, Nam-Cheol; Desjardins, Anne E.; Wu, Christine D.; Kinghorn, A. Douglas
CORPORATE SOURCE: Program for Collaborative Research in the Pharmaceutical Sciences and Department of Medicinal Chemistry and Pharmacognosy College of Pharmacy, University of Illinois, Chicago, IL, 60612, USA
SOURCE: Journal of Natural Products (1999), 62(10), 1379-1384
CODEN: JNPRDF; ISSN: 0163-3864
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Four new triterpenoid glycosides were isolated from the root bark of Mussaenda macrophylla. Their structures were detd. as 3-O-.beta.-D-glucopyranosyl-28-O-.alpha.-L-rhamnopyranosyl-16.alpha.-hydroxy-23-deoxyprotobassic acid (1), 28-O-.beta.-D-glucopyranosyl-16.alpha.-hydroxy-23-deoxyprotobassic acid (2), 3-O-.beta.-D-glucopyranosyl-28-O-.alpha.-L-rhamnopyranosyl-16.alpha.-hydroxyprotobassic acid (3), and 3-O-{[.beta.-D-glucopyranosyl-(1.fwdarw.6)]-O-.alpha.-L-rhamnopyranosyl-(1.fwdarw.2)-O-.beta.-D-glucopyranosyl-(1.fwdarw.2)}-O-.beta.-D-glucopyranosyl-(1.fwdarw.3)-O-.beta.-D-glucopyranosyl-cycloarta-22,24-dien-27-oic acid (mussaendoside W, 4). Four known triterpenoids [3-O-acetyloleanolic acid (5), 3-O-acetyldaturadiol (6), rotundic acid (7), and 16.alpha.-hydroxyprotobassic acid (8)] were also isolated. The structures of 1-4 were detd. by several spectroscopic techniques including 2D NMR methods. Compds. 1-6 showed inhibitory activity against a periodontopathic bacterium, Porphyromonas gingivalis, but were inactive against the cariogenic organism, Streptococcus mutans.

IT **248912-10-9P**, Mussaendoside W
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); PREP (Preparation)
(activity of triterpenoid glycosides from the root bark of Mussaenda

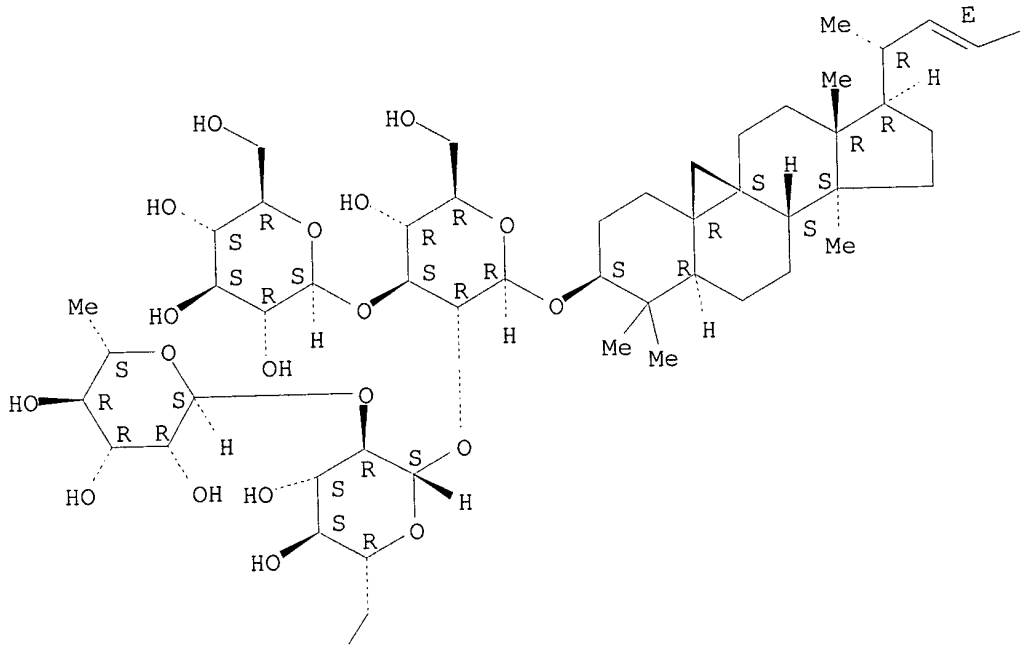
macrophylla against two oral pathogens)

RN 248912-10-9 HCAPLUS

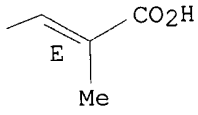
CN 9,19-Cyclolanosta-22,24-dien-26-oic acid, 3-[(O-6-deoxy-.alpha.-L-mannopyranosyl-(1.fwdarw.2)-O-[.beta.-D-glucopyranosyl-(1.fwdarw.6)]-O-.beta.-D-glucopyranosyl-(1.fwdarw.2)-O-[.beta.-D-glucopyranosyl-(1.fwdarw.3)]-.beta.-D-glucopyranosyl)oxy]-, (3.beta.,22E,24E)- (9CI) (CA INDEX NAME)

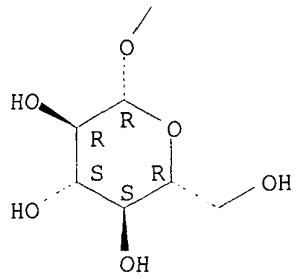
Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A



PAGE 1-B





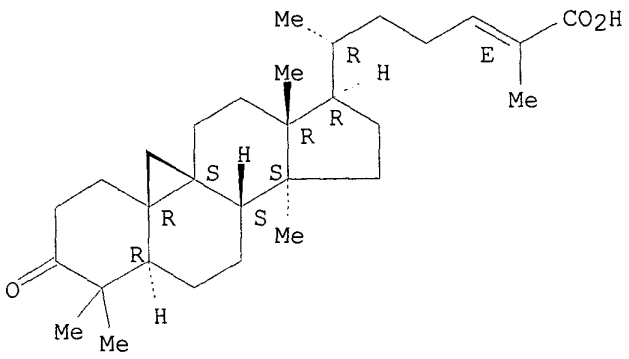
REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 4 OF 16 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1999:532419 HCAPLUS
DOCUMENT NUMBER: 131:283964
TITLE: Resveratrol tetramers from Vatica diospyroides
AUTHOR(S): Seo, Eun-Kyoung; Chai, Heebyung; Constant, Howard L.; Santisuk, Thawatchai; Reutrakul, Vichai; Beecher, Christopher W. W.; Farnsworth, Norman R.; Cordell, Geoffrey A.; Pezzuto, John M.; Kinghorn, A. Douglas
CORPORATE SOURCE: Program for Collaborative Research in the Pharmaceutical Sciences and Department of Medicinal Chemistry and Pharmacognosy, College of Pharmacy University of Illinois at Chicago, Chicago, IL, 60612, USA
SOURCE: Journal of Organic Chemistry (1999), 64(19), 6976-6983
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Vatdiospyroidol (I), a novel cytotoxic resveratrol tetramer, was isolated from the stems of Vatica diospyroides Sym. (Dipterocarpaceae) by bioassay-guided fractionation monitored with a human oral epidermoid carcinoma (KB) cell line. Another novel resveratrol tetramer, vaticaphenol A (II), was obtained as a noncytotoxic constituent, along with the known compds., bergenin, betulin, betulinic acid, mangiferonic acid, and (E)-resveratrol 3-O-.beta.-D-glucopyranoside. The structures of compds. I and II were elucidated by spectral anal., including 1D and 2D NMR expts., and by mol. modeling.

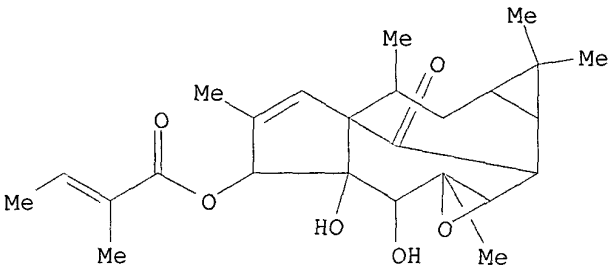
IT **13878-90-5**, Mangiferonic acid
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)
(from Vatica diospyroides)
RN 13878-90-5 HCAPLUS
CN 9,19-Cyclolanost-24-en-26-oic acid, 3-oxo-, (24E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



REFERENCE COUNT: 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 5 OF 16 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1999:4251 HCAPLUS
DOCUMENT NUMBER: 130:34353
TITLE: Dietary cancer risk conditional cancerogens in produce of livestock fed on species of spurge (Euphorbiaceae). Part 1. Skin irritant and **tumor**-promoting ingenane-type diterpene esters in E. peplus, one of several herbaceous Euphorbia species contaminating fodder of livestock. [Erratum to document cited in CA129:312034]
AUTHOR(S): Zayed, Salah M. A. D.; Farghaly, Madiha; Taha, Hamby; Gotta, Hubert; Hecker, Erich
CORPORATE SOURCE: Laboratory Organic Chemistry, National Research Center, Cairo, Egypt
SOURCE: Journal of Cancer Research and Clinical Oncology (1998), 124(6), 351
CODEN: JCROD7; ISSN: 0171-5216
PUBLISHER: Springer-Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
AB On page 135, in Table 2, the words "Low" in the last column should read "Medium"; the complete column is reprinted.
IT **214771-74-1P**
RL: ADV (Adverse effect, including toxicity); BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(skin irritant and **tumor**-promoting ingenane-type diterpene esters in Euphorbia (Erratum))
RN 214771-74-1 HCAPLUS
CN 2-Butenoic acid, 2-methyl-, (1aS,2R,2aR,3aR,5R,5aS,8S,8aS,9S,9aR)-1a,2,2a,3a,4,5,8,8a,9,9a-decahydro-8a,9-dihydroxy-3,3,5,7,9a-pentamethyl-10-oxo-3H-2,5a-methanocyclopenta[4,5]cyclopropa[8,9]cyclodec[1,2-b]oxiren-8-yl ester, (2Z)- (9CI) (CA INDEX NAME)

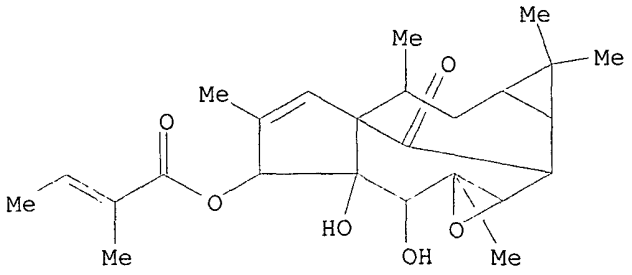


L22 ANSWER 6 OF 16 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1998:577094 HCAPLUS
DOCUMENT NUMBER: 129:312034
TITLE: Dietary cancer risk conditional cancerogens in produce of livestock fed on species of spurge (Euphorbiaceae). Part 1. Skin irritant and **tumor**-promoting ingenane-type diterpene esters in E. peplus, one of several herbaceous Euphorbia species contaminating fodder of livestock
AUTHOR(S): Zayed, Salah M. A. D.; Farghaly, Madiha; Taha, Hamdy; Gotta, Hubert; Hecker, Erich
CORPORATE SOURCE: Laboratory Organic Chemistry, National Research Center, Cairo, Egypt
SOURCE: Journal of Cancer Research and Clinical Oncology (1998), 124(3/4), 131-140
CODEN: JCROD7; ISSN: 0171-5216
PUBLISHER: Springer-Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Several herbaceous plants of the genus Euphorbia, widespread as weeds and contaminants of livestock fodder, were identified botanically and exts. of their aerial parts were tested for irritancy on the mouse ear. As compared to a std. probe of croton oil, the exts. of E. peplus, E. nubica, and E. helioscopia displayed irritancy. The most active ext. (that from E. peplus) was investigated by a fractionation procedure monitored by the mouse ear assay, and 5 molecularly uniform irritant E. factors Pe1-Pe5 were identified as diterpene ester-type toxins. Together these factors comprise at least 11 ppm in the aerial parts. They were characterized individually to carry the diterpene parent alcs. ingenol, 20-deoxyingenol, and 20-deoxyingenol-6.alpha.,7.alpha.-epoxide. The irritancy of the aerial plant parts was caused mainly by the E. factors Pe1 and Pe2 together. Upon chronic administration of these irritants and hyperplasiogens as principal cancerogenic risk factors in the mouse skin initiation/promotion bioassay, Pe1 and Pe2 were established as **tumor** promoters.

IT **214771-74-1P**
RL: ADV (Adverse effect, including toxicity); BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(skin irritant and **tumor**-promoting ingenane-type diterpene esters in Euphorbia)
RN 214771-74-1 HCAPLUS
CN 2-Butenoic acid, 2-methyl-, (1aS,2R,2aR,3aR,5R,5aS,8S,8aS,9S,9aR)-1a,2,2a,3a,4,5,8,8a,9,9a-decahydro-8a,9-dihydroxy-3,3,5,7,9a-pentamethyl-10-oxo-3H-2,5a-methanocyclopenta[4,5]cyclopropa[8,9]cyclodec[1,2-b]oxiren-

8-yl ester, (2Z)- (9CI) (CA INDEX NAME)



L22 ANSWER 7 OF 16 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1997:443284 HCAPLUS
DOCUMENT NUMBER: 127:70830
TITLE: Isolation of triterpene acids from Kadsura japonica as anti-androgen agents
INVENTOR(S): Hayashi, Katsuhiro; Suzuki, Tatsuhiko; Oishi, Seiko; Yagi, Kunio; Koda, Mayumi; Kakita, Shingo; Yokoo, Yoshiharu; Honda, Shinkichi; Tadano, Toshio
PATENT ASSIGNEE(S): Kyowa Hakko Kogyo Co., Ltd., Japan; Kyowa Medex Co., Ltd.; Oyo Seikagaku Kenkyusho K. K.
SOURCE: Jpn. Kokai Tokkyo Koho, 9 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 09151196	A2	19970610	JP 1993-171671	19930712
JP 3260918	B2	20020225		

OTHER SOURCE(S): MARPAT 127:70830
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

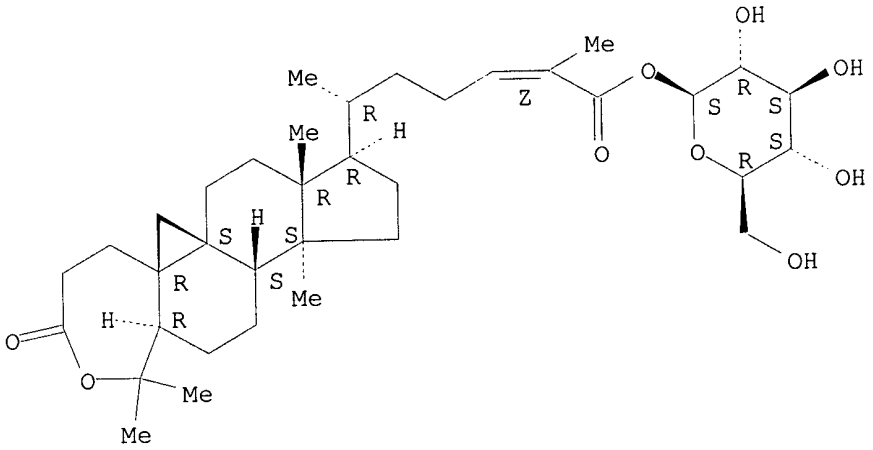
AB The title compds. (I; X = O, single bond; R = H, OH) are isolated by extn. from Kadsura japonica using alcs. I are useful as anti-androgen agents for prevention and treatment of hair diseases such as male hair loss, prostatic hypertrophy, prostatic cancer, and related diseases. The title compd. (II) showed IC50 of 4.3 X 10-8 M against androgen receptor binding activity. Formulation contg. II is presented.

IT **190836-57-8P 190836-60-3P 190836-64-7P**
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); PUR (Purification or recovery); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(isolation of triterpene acids from Kadsura japonica as anti-androgen agents)

RN 190836-57-8 HCAPLUS
CN .beta.-D-Glucopyranose, 1-[(2Z,6R)-6-[(5aR,6aS,8aR,9R,11aS,11bS,13aR)-

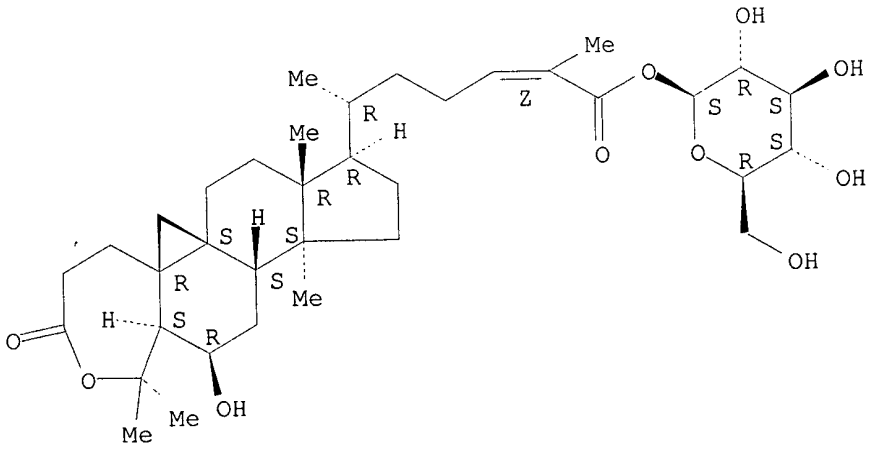
tetradecahydro-1,1,8a,11a-tetramethyl-3-oxo-3H,6H-cyclopenta[5,6]cyclopropa[1,8a]naphth[2,1-c]oxepin-8-yl]-2-methyl-2-heptenoate] (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



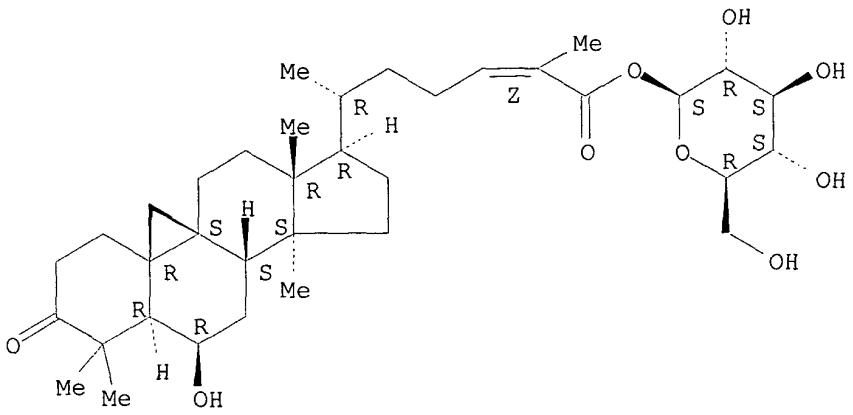
RN 190836-60-3 HCAPLUS
CN .beta.-D-Glucopyranose, 1-[(2Z,6R)-6-[(5aR,6aS,8aR,9R,11aS,11bS,13R,13aS)-tetradecahydro-13-hydroxy-1,1,8a,11a-tetramethyl-3-oxo-3H,6H-cyclopenta[5,6]cyclopropa[1,8a]naphth[2,1-c]oxepin-8-yl]-2-methyl-2-heptenoate] (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



RN 190836-64-7 HCAPLUS
CN 9,19-Cyclolanost-24-en-26-oic acid, 6-hydroxy-3-oxo-, .beta.-D-glucopyranosyl ester, (6.beta.,24Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.



L22 ANSWER 8 OF 16 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1996:618612 HCAPLUS
DOCUMENT NUMBER: 125:257163
TITLE: Antiandrogenic triterpenes and their extraction from Kadsura japonica
INVENTOR(S): Hayashi, Katsuhiro; Suzuki, Tatsuhiko; Ooishi, Shigeko; Yagi, Kunio; Koda, Mayumi; Kakita, Shingo; Yokoo, Yoshiharu; Pponda, Shinkichi; Tadano, Toshio
PATENT ASSIGNEE(S): Kyowa Hakko Kogyo Kk, Japan; Kyowa Medex Co Ltd; Oyo Seikagaku Kenkyusho
SOURCE: Jpn. Kokai Tokkyo Koho, 8 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 08193094	A2	19960730	JP 1995-3025	19950112

OTHER SOURCE(S): MARPAT 125:257163

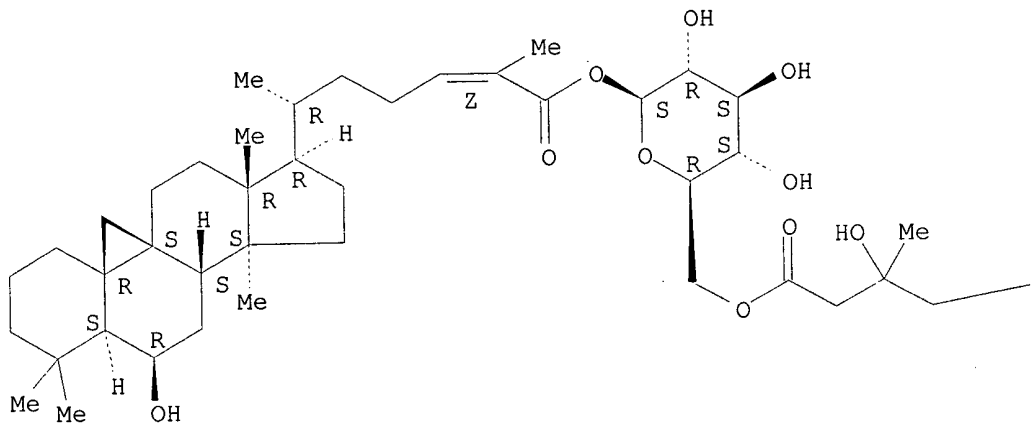
AB Novel antiandrogenic triterpenes and their extn. from K. japonica are claimed. Two compds. extd. from K. japonica are purified and characterized by spectrochem. and other methods. For dosage form prepns., 2 mg of the antiandrogenic triterpene was dissolved in 100 mL ethanol, mixed with 10 mg dextrin, and dried. Capsules were formulated contg. the powder 3, lactose 121, corn starch 50 and hydroxypropyl cellulose 16 mg.

IT **182123-23-5P 182123-26-8P**
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); PUR (Purification or recovery); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(novel antiandrogenic triterpenes and their extn. from Kadsura japonica)

RN 182123-23-5 HCAPLUS
CN 9,19-Cyclolanost-24-en-26-oic acid, 6-hydroxy-, 6-O-(4-carboxy-3-hydroxy-3-methyl-1-oxobutyl)-.beta.-D-glucopyranosyl ester, (6.beta.,24Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A



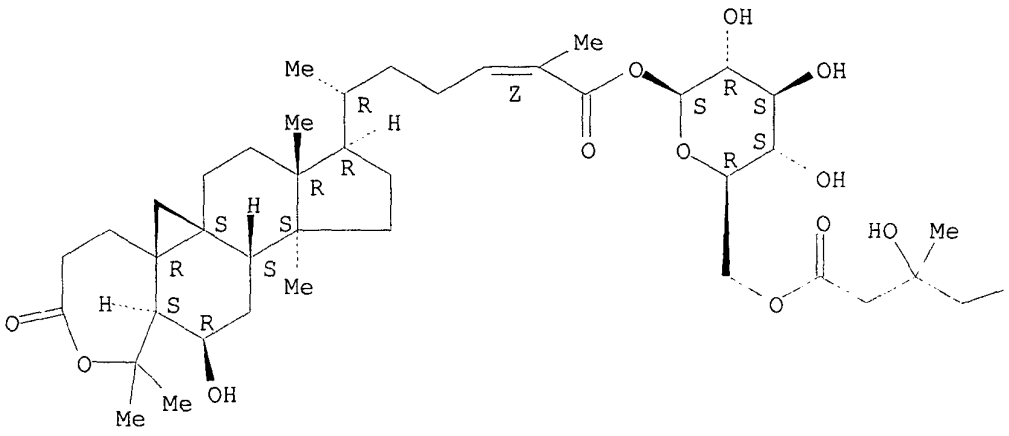
PAGE 1-B

—CO_2H

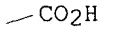
RN 182123-26-8 HCAPLUS
CN .beta.-D-Glucopyranose, 6-O-(4-carboxy-3-hydroxy-3-methyl-1-oxobutyl)-, 1-[(2Z,6R)-6-[(5aR,6aS,8aR,9R,11aS,11bS,13R,13aS)-tetradecahydro-13-hydroxy-1,1,8a,11a-tetramethyl-3-oxo-3H,6H-cyclopenta[5,6]cyclopropa[1,8a]naphth[2,1-c]oxepin-8-yl]-2-methyl-2-heptenoate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A



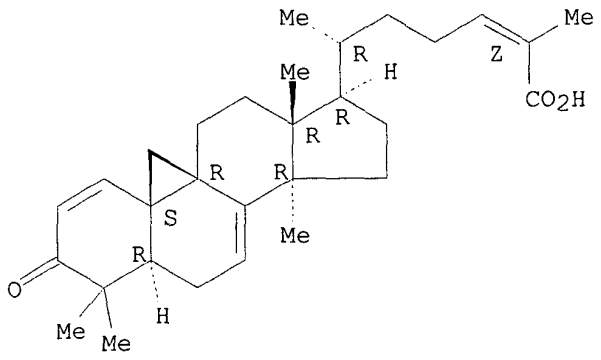
PAGE 1-B



L22 ANSWER 9 OF 16 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1996:437039 HCAPLUS
DOCUMENT NUMBER: 125:132052
TITLE: Analgesic and anti-**inflammatory** activity of tetracyclic triterpenoids isolated from Pistacia integerrima galls
AUTHOR(S): Ansari, S. H.; Ali, M.
CORPORATE SOURCE: Fac. Pharmacy, Jamia Hamdard, New Delhi, 110062, India
SOURCE: Fitoterapia (1996), 67(2), 103-105
CODEN: FTRPAE; ISSN: 0367-326X
PUBLISHER: Inverni della Beffa SpA
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The analgesic and anti-**inflammatory** activity of six tetracyclic triterpenoids, pistacigerrimones A, B, C, D, E and F, isolated from the galls of P. integerrima was studied. Pistacigerrimones C and D gave highly significantly results.
IT **158372-26-0**, Pistacigerrimone F
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); **THU (Therapeutic use)**; BIOL (Biological study); USES (Uses)
(analgesic and anti-**inflammatory** activity of tetracyclic

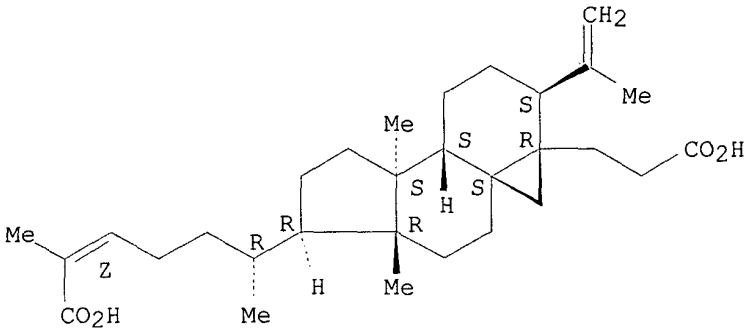
triterpenoids isolated from Pistacia integerrima galls)
RN 158372-26-0 HCAPLUS
CN 9,19-Cyclolanosta-1,7,24-trien-26-oic acid, 3-oxo-, (24Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



L22 ANSWER 10 OF 16 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1996:265316 HCAPLUS
DOCUMENT NUMBER: 124:284381
TITLE: Nigranoic Acid, a Triterpenoid from Schisandra sphaerandra That Inhibits HIV-1 Reverse Transcriptase
AUTHOR(S): Sun, Han-dong; Qiu, Sheng-xiang; Lin, Long-ze; Wang, Zong-yu; Lin, Zhong-wen; Pengsuparp, Thitima; Pezzuto, John M.; Fong, Harry H. S.; Cordell, Geoffrey A.; Farnsworth, Norman R.
CORPORATE SOURCE: Kunming Institute of Botany, Chinese Academy of Sciences, Kunming, 650204, Peop. Rep. China
SOURCE: Journal of Natural Products (1996), 59(5), 525-7
CODEN: JNPRDF; ISSN: 0163-3864
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB An A ring-secocycloartene triterpenoid, nigranoic acid (3,4-secocycloarta-4(28),24-(Z)-diene-3,26-dioic acid), was isolated from the stems of Schisandra sphaerandra, a Chinese traditional medicinal plant. Its structure elucidation and unambiguous NMR spectral assignment were achieved by the combination of 1D- and 2D-NMR techniques with the aid of computer modeling. Nigranoic acid showed activity in several anti-HIV reverse transcriptase and polymerase assays.
IT **39111-07-4**, Nigranoic Acid
RL: **BAC (Biological activity or effector, except adverse)**; BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)
(nigranoic acid triterpenoid from Schisandra sphaerandra inhibitor of HIV-1 Reverse Transcriptase)
RN 39111-07-4 HCAPLUS
CN 1H-Cyclopenta[a]cyclopropa[e]naphthalene-3a(4H)-propanoic acid, 7-[(1R,4Z)-5-carboxy-1-methyl-4-hexenyl]decahydro-6a,9a-dimethyl-3-(1-methylethenyl)-, (3S,3aR,4aS,6aR,7R,9aS,9bS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



L22 ANSWER 11 OF 16 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1991:531979 HCAPLUS
DOCUMENT NUMBER: 115:131979
TITLE: Isolation and structures of schisanlactone E and changnanic acid
AUTHOR(S): Liu, Jiasen; Huang, Meifen
CORPORATE SOURCE: Shanghai Inst. Mater. Med., Acad. Sin., Shanghai, 200031, Peop. Rep. China
SOURCE: Huaxue Xuebao (1991), 49(5), 502-6
CODEN: HHHPA4; ISSN: 0567-7351
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
GI

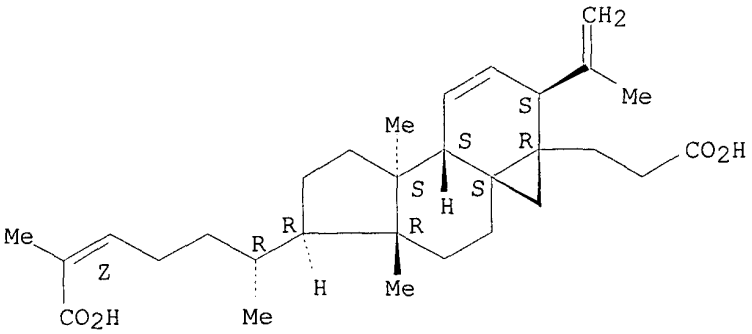
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Two new triterpenoid compds., schisanlactone E (I) and changnanic acid (II), along with three known compds., schisanlactone B (III), meso-dihydroguaiaretic acid and .beta.-sitosterol, were isolated from the root bark of Kadsura longipedunculata Finet. et Gagnep. indigenous to the Lin-An district in Zhejiang province of China. Their structures were elucidated by spectroscopic studies. In an anticancer screening I and II show significant inhibition of **leukemia** p-388 cells in vitro (IC50 1 .mu.g/mL and 10 .mu.g/mL resp.).

IT **136040-44-3**
RL: BIOL (Biological study)
(of Kadsura longipedunculata, isolation, mol. structure and **neoplasm** inhibiting activity of)

RN 136040-44-3 HCAPLUS
CN 3H-Cyclopenta[a]cyclopropa[e]naphthalene-3a(4H)-propanoic acid, 7-[(1R,4Z)-5-carboxy-1-methyl-4-hexenyl]-5,6,6a,7,8,9,9a,9b-octahydro-6a,9a-dimethyl-3-(1-methylethenyl)-, (3S,3aR,4aS,6aR,7R,9aS,9bS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



L22 ANSWER 12 OF 16 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1991:489129 HCAPLUS
DOCUMENT NUMBER: 115:89129
TITLE: Isolation and structures of schisantherin J and schisanlactone F
AUTHOR(S): Liu, Jiasen; Pan, Yanping
CORPORATE SOURCE: Shanghai Inst. Mater. Med., Chin. Acad. Sci., Shanghai, 200031, Peop. Rep. China
SOURCE: Huaxue Xuebao (1991), 49(3), 308-12
CODEN: HHHPA4; ISSN: 0567-7351
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
GI

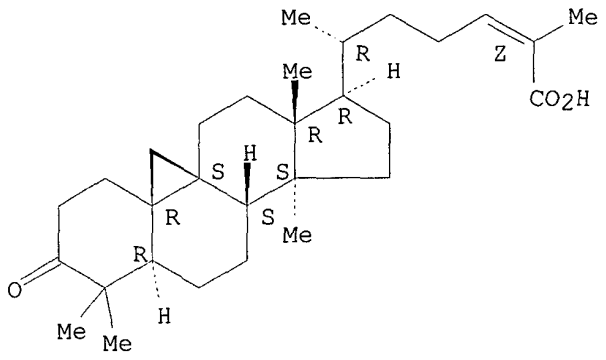
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB One new lignan, schisantherin J(I) and one new triterpenoid, schisanlactone F (II) were isolated along with four known compds., schisanlactone A, schizandronic acid, epianwuweizic acid and di-Me deangeloyl schisantherin F, from the seed of Kadsura longipeduaculata Finet. et Gagnep. Their structures including abs. configurations were elucidated by spectroscopic studies and chem. conversions. In anticancer screening, II shows a significant inhibition of **leukemia** P-388 cells in vitro (ED50 5 .mu.g/mL).

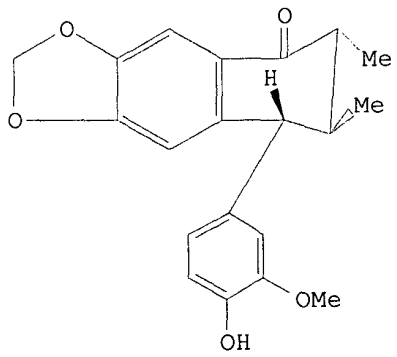
IT **55511-14-3**, Schisandronic acid
RL: PROC (Process)
(isolation of, from Kadsura longipedunculata)

RN 55511-14-3 HCAPLUS
CN 9,19-Cyclolanost-24-en-26-oic acid, 3-oxo-, (24Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



L22 ANSWER 13 OF 16 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1988:489752 HCAPLUS
DOCUMENT NUMBER: 109:89752
TITLE: Studies on the constituents of Schisandraceae plants in Shennongjia District. I. Constituents of Schisandra propinqua Hook. F. et Thoms. var. sinensis Oliv
AUTHOR(S): Liu, Jiasen; Ma, Yuting; Huang, Meifen
CORPORATE SOURCE: Shanghai Inst. Mater. Med., Acad. Sin., Shanghai, Peop. Rep. China
SOURCE: Huaxue Xuebao (1988), 46(4), 345-8
CODEN: HHHPA4; ISSN: 0567-7351
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
OTHER SOURCE(S): CASREACT 109:89752
GI

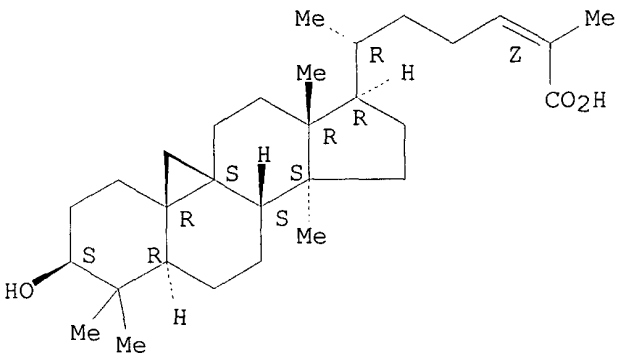


I

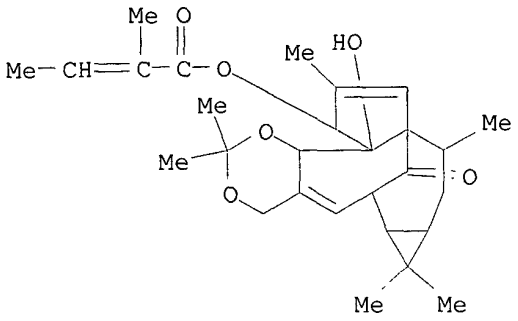
AB Six compds. were isolated from the stems and roots of S. propinqua var. sinensis. One is a new lignan named epienshicine (I), m.p. 163-164.degree., [.alpha.]D11.5 -18.2.degree. (CHCl3), which was shown to be 1-oxy-2R,3S-dimethyl-4R-(3-methoxy-4-hydroxyphenyl)-6,7-methylenedioxytetralin by means of spectral anal. and chem. transformation into (+)-galcatin. The remaining five compds. were identified as enshicine, isoschisandrolic acid (II), deoxyschizandrin, .beta.-sitosterol, and stearic acid, in which II is isolated from the natural resources for the first time. I shows activity against **leukemia** P-388 in vitro.

IT **55511-17-6**
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)
(of Schisandra propinqua)
RN 55511-17-6 HCAPLUS
CN 9,19-Cyclolanost-24-en-26-oic acid, 3-hydroxy-, (3.beta.,24Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



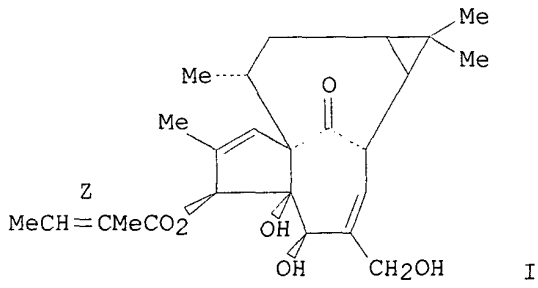
L22 ANSWER 14 OF 16 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1984:507324 HCAPLUS
DOCUMENT NUMBER: 101:107324
TITLE: On the active principles of the Euphorbiaceae, IX. Ingenane type diterpene esters from five Euphorbia species
AUTHOR(S): Gotta, H.; Adolf, W.; Opferkuch, H. J.; Hecker, E.
CORPORATE SOURCE: Inst. Biochem., Dtsch. Krebsforschungszent., Heidelberg, D-6900, Fed. Rep. Ger.
SOURCE: Zeitschrift fuer Naturforschung, Teil B: Anorganische Chemie, Organische Chemie (1984), 39B(5), 683-94
CODEN: ZNBAD2; ISSN: 0340-5087
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Investigation of E. antiquorum, E. helioscopia, E. palustris, E. peplus, and E. quadrialata for irritant and **tumor**-promoting constituents afforded several new ingenane diterpene esters derived from the parent alcs. ingenol and 20-deoxyingenol and from the hitherto unknown 20-deoxy-16-hydroxyingenol and 20-deoxy-13,16-dihydroxyingenol. The irritant activities of the natural compds. are reported, together with some aspects on structure activity relationships.
IT **87980-68-5**
RL: BIOL (Biological study)
(from Euphorbia species)
RN 87980-68-5 HCAPLUS
CN 2-Butenoic acid, 2-methyl-, 6,6a,7a,8,9,12,12a,12b-octahydro-12a-hydroxy-2,2,7,7,9,11-hexamethyl-13-oxo-7H-6,9a-methano-4H-cyclopenta[9,10]cyclopropa[5,6]cyclodeca[1,2-d]-1,3-dioxin-12-yl ester, [6R-[6.alpha.,6a.alpha.,7a.alpha.,9.alpha.,9a.alpha.,12.beta.(Z),12a.beta.,12b.alpha.]]- (9CI) (CA INDEX NAME)



IT **91413-77-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 91413-77-3 HCAPLUS
CN 2-Butenoic acid, 2-methyl-, 1a,2,3,9,12,12a-hexahydro-1,1,3,5,7,7,10-heptamethyl-13-oxo-5aH-3a,12-methano-1H-cyclopropa[5',6']cyclodeca[1',2':1,5]cyclopenta[1,2-d][1,3]dioxol-9-yl ester, [1aR-[1a.alpha.,3.alpha.,3a.alpha.,5a.alpha.,8aR*,9.beta.(Z),12.beta.,12a.alpha.]]- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

L22 ANSWER 15 OF 16 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1984:12496 HCAPLUS
DOCUMENT NUMBER: 100:12496
TITLE: 3-O-Angeloylingenol, the toxic and skin irritant factor from latex of Euphorbia antiquorum L. (Euphorbiaceae) and from a derived Thai purgative and anthelimintic (vermifuge) drug
AUTHOR(S): Adolf, W.; Chanai, S.; Hecker, E.
CORPORATE SOURCE: Inst. Biochem., Dtsch. Krebsforschungszent., Heidelberg, D-6900, Fed. Rep. Ger.
SOURCE: Journal of the Science Society of Thailand (1983), 9(2), 81-8
CODEN: VKSTDB; ISSN: 0303-8122
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



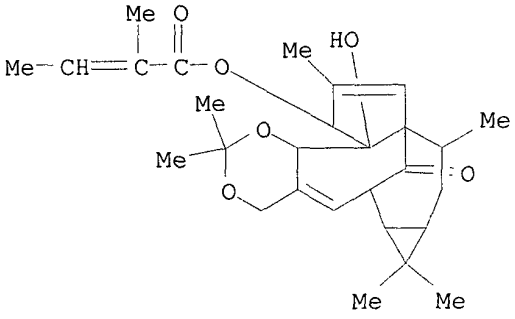
I

AB From a latex of E. antiquorum, as well as from the purgative and anthelmintic (vermifuge) Thai drug yang Sa-Lad-Dai (dried, powd. latex), the highly skin irritant and toxic Euphorbia factor An1 3-O-angeloylingenol (I) [75567-37-2] was isolated by combination of countercurrent distributions and chromatog. Because of the acute toxicity of I and of the possible risk of **cocarcinogenesis** by **tumor** promotion, utilization of drugs made up from dried or fresh latex as practiced in Thailand in purgatives and vermifuges should be abandoned.

IT **87980-68-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 87980-68-5 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, 6,6a,7a,8,9,12,12a,12b-octahydro-12a-hydroxy-2,2,7,7,9,11-hexamethyl-13-oxo-7H-6,9a-methano-4H-cyclopenta[9,10]cyclopropa[5,6]cyclodeca[1,2-d]-1,3-dioxin-12-yl ester, [6R-[6.alpha.,6a.alpha.,7a.alpha.,9.alpha.,9a.alpha.,12.beta.(Z),12a.beta.,12b.alpha.]]- (9CI) (CA INDEX NAME)



L22 ANSWER 16 OF 16 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1983:12688 HCAPLUS

DOCUMENT NUMBER: 98:12688

TITLE: On the active principles of the spurge family (Euphorbiaceae). IV. Skin irritant and **tumor** promoting diterpene esters from Euphorbia ingens E. Mey

AUTHOR(S): Opferkuch, H. J.; Hecker, E.

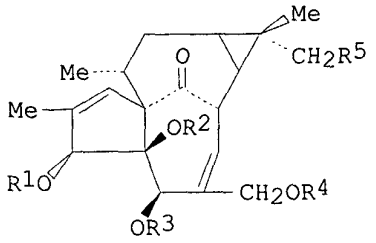
CORPORATE SOURCE: Inst. Biochem., Dtsch. Krebsforschungszent., Heidelberg, D-6900/1, Fed. Rep. Ger.

SOURCE: Journal of Cancer Research and Clinical Oncology (1982), 103(3), 255-68
CODEN: JCROD7; ISSN: 0171-5216

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



I

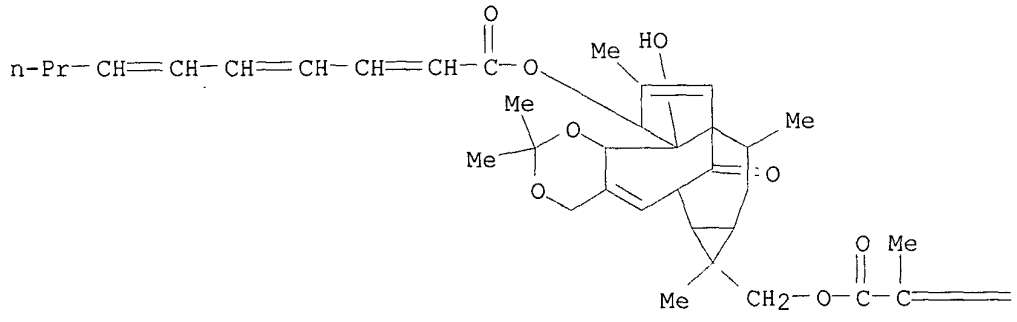
AB The irritant and **tumor**-promoting principles of the latex of Euphorbia ingens were isolated together with several nonirritant compds. The Euphorbia factor I1 [52557-26-3], I5 [52557-27-4], and I6 [52557-28-5] are esters of ingenane-type polyfunctional diterpene alcs. (I). Euphorbia factor I1 is characterized as the 3-hexadecanoate of I and Euphorbia factor I6 as the 3-deca-2.4.6-trienoic acid ester of I. Euphorbia factor I5 is the 16-angelate-3-deca-2.4.6-trienoate of 16-hydroxyingenol. Nonirritant diterpenes of the latex are I2 [39071-33-5], the ingenol-20-hexadecanoate - an isomer of Euphorbia factor I1 - and I4, the 3.7.12-triacetate-8-nicotinate of the macrocyclic lathyrane-type polyfunctional diterpene alc. ingol. The diterpene alcs. ingenol and 16-hydroxyingenol are inactive as irritants and **tumor** promoters of mouse skin. Compared to croton oil factor A1, the Euphorbia factor I1 exhibits .apprx.1/10 of the irritant and **tumor** -promoting activity in mouse skin. I1 shows no reasonable **tumorigenic** activity. Compared with I1, Euphorbia factors I5 and I6 are more potent irritants and less potent **tumor** promoters.

IT **83919-97-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and dealkylation of)

RN 83919-97-5 HCAPLUS

CN 2,4,6-Decatrienoic acid, 6,6a,7,7a,8,9,12a,12b-octahydro-12a-hydroxy-2,2,7,9,11-pentamethyl-7-[[(2-methyl-1-oxo-2-butenyl)oxy]methyl]-13-oxo-12H-6,9a-methano-4H-cyclopenta[9,10]cyclopropa[5,6]cyclodeca[1,2-d]-1,3-dioxin-12-yl ester, [6R-(6.alpha.,6a.alpha.,7.alpha.,7a.alpha.,9.alpha.,9a.alpha.,12.beta.,12a.beta.,12b.alpha.)]- (9CI) (CA INDEX NAME)

PAGE 1-A



=CH-Me

=> d ibib abs

L26 ANSWER 1 OF 1 TOXCENTER COPYRIGHT 2002 ACS

ACCESSION NUMBER:	1993:975 TOXCENTER
COPYRIGHT:	Copyright 2002 ASHP
DOCUMENT NUMBER:	30-12301
TITLE:	Skin irritant principle from Euphorbia griseola
AUTHOR(S):	Gundidza, M.; Sorg, B.; Hecker, E.
CORPORATE SOURCE:	Germany Cancer Res. Ctr., Inst. of Biochem., Im Neuenheimer Feld 280, D-6900 Heidelberg, Germany
SOURCE:	International Pharmacy Journal (Netherlands), (Jan-Feb 1993) Vol. 7, pp. 19-21. 13 Refs CODEN: IPHJEN. ISSN: 1010-0423.
DOCUMENT TYPE:	Journal
FILE SEGMENT:	IPA
OTHER SOURCE:	IPA 93:3196
LANGUAGE:	English
SUMMARY LANGUAGE:	French; German; Spanish
ENTRY DATE:	Entered STN: 20011116 Last Updated on STN: 20011116

AB **Euphorbia factor EG1**, a diterpene of the ingenane-type parent alcohol with angelic acid as the acid substituent, was isolated from Euphorbia griseola and its irritant activity was studied using the mouse ear test. The skin irritant activity of the compound 24 h after administration was found to be 0.348 n mole/ear.
Ellen Katz Neumann

L23 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2002 ACS
RN 157807-48-2 REGISTRY
CN Euphorbia factor EG1 (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1H-2,8a-Methanocyclopenta[a]cyclopropa[e]cyclodecene, euphorbia factor EG1 deriv.
OTHER NAMES:
CN 1H-2,8a-Methanocyclopenta[a]cyclopropa[e]cyclodecen-11-one, 1a,2,5,5a,6,9,10,10a-octahydro-5,5a,6-trihydroxy-4-(hydroxymethyl)-1,1,7,9-tetramethyl-, mono[(Z)-2-methyl-2-butenoate], (1aR,2S,5R,5aR,6S,8aS,9R,10aR)-
CN Ingenol monoangelate
FS STEREOSEARCH
MF C25 H34 O6
CI IDS
SR American Society of Hospital Pharmacists

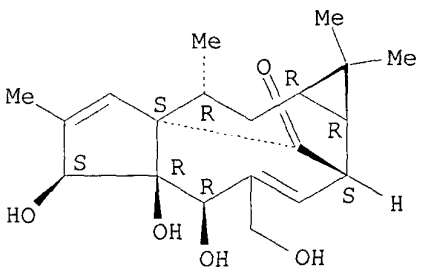
Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C3-C5-C7-C7	C3-C5-C7-C7	3-5-7-7	C15	2809.1.1	1 in CM 1

CM 1

CRN 30220-46-3
CMF C20 H28 O5

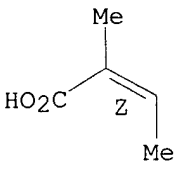
Absolute stereochemistry.



CM 2

CRN 565-63-9
CMF C5 H8 O2

Double bond geometry as shown.


Me
HO2C
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Me

=>

=> d ibib abs

L32 ANSWER 1 OF 2 TOXCENTER COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1975:71877 TOXCENTER
COPYRIGHT: Copyright 2002 ACS
DOCUMENT NUMBER: CA08221133804E
TITLE: Diterpene esters from Euphorbium and their irritant and cocarcinogenic activity
AUTHOR(S): Hergenhahn, M.; Kusumoto, S.; Hecker, E.
CORPORATE SOURCE: Dtsch. Krebsforschungszent., Inst. Biochem., Heidelberg.
SOURCE: Experientia, (1974) Vol. 30, No. 12, pp. 1438-40.
CODEN: EXPEAM.
DOCUMENT TYPE: Journal
FILE SEGMENT: CAPLUS
OTHER SOURCE: CAPLUS 1975:133804
LANGUAGE: English
ENTRY DATE

AB Diterp
resini
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L32 & 34 came from some text searching - still nothing really for using this stuff to treat cancer

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42.3,

=> d ibib abs 2

L32 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1975:133804 CAPLUS
DOCUMENT NUMBER: 82:133804
TITLE: Diterpene esters from Euphorbium and their irritant and cocarcinogenic activity
AUTHOR(S): Hergenhahn, M.; Kusumoto, S.; Hecker, E.
CORPORATE SOURCE: Dtsch. Krebsforschungszent., Inst. Biochem., Heidelberg, Ger.
SOURCE: Experientia (1974), 30(12), 1438-40
CODEN: EXPEAM
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB Diterpene esters were obtained from air-dried latex of Euphorbia resinifera. The 3-hr irritant dose 50 (ID50) was 0.18 nmole/mouse ear for 12-deoxyphorbol-13-**angelate**-20-acetate (I) [25090-72-6], 0.024 nmole/ear for 12-deoxyphorbol-13-isobutyrate-20-acetate (II) [25090-71-5], and 0.0027 nmole/ear for 12-deoxyphorbol-13-phenylacetate-20-acetate (III) [54662-30-5]. Two ingol esters were not irritant. Percentage of **tumor** bearers among surviving mice, **treated** topically with 0.2 .mu.mole I, 0.2 II, 0.1 III, and 0.1 **ingenol** 3-acylate mixt., twice weekly for 12 weeks, following **tumor** initiation by 0.1 .mu.mole 7,12-dimethylbenz[a]anthracene, was 11.1, 0, 7.4, and 42.3, resp.

=> d ibib abs 1-10

L34 ANSWER 1 OF 10 MEDLINE

ACCESSION NUMBER: 2000280699 MEDLINE
DOCUMENT NUMBER: 20280699 PubMed ID: 10821064
TITLE: Diterpenoids from Euphorbia peplus.
AUTHOR: Hohmann J; Evanics F; Berta L; Bartok T
SOURCE: PLANTA MEDICA, (2000 Apr) 66 (3) 291-4.
Journal code: 0066751. ISSN: 0032-0943.
PUB. COUNTRY: GERMANY: Germany, Federal Republic of
DOCUMENT TYPE: Letter
LANGUAGE: English
FILE SEGMENT: Priority Journals
ENTRY MONTH: 200006
ENTRY DATE: Entered STN: 20000706
Last Updated on STN: 20000706
Entered Medline: 20000626

AB From a pro-**inflammatory** active extract of Euphorbia peplus, two new diterpene polyesters based on the pepluane and jatrophane skeletons were isolated, together with four known **ingenane** and jatrophane diterpenes. The structures were determined on the basis of extensive NMR studies. **Ingenol** 3-**angelate**, which was obtained for the first time from this plant, is an irritant toxin with high activity.

L34 ANSWER 2 OF 10 TOXCENTER COPYRIGHT 2002 ACS DUPLICATE 1
ACCESSION NUMBER: 2000:146716 TOXCENTER
COPYRIGHT: Copyright 2002 ACS
DOCUMENT NUMBER: CA13307086701D
TITLE: Diterpenoids from Euphorbia peplus
AUTHOR(S): Hohmann, Judit; Evanics, Ferenc; Berta, Laszlo; Bartok, Tibor
CORPORATE SOURCE: Department of Pharmacognosy, Albert Szent-Gyorgyi Medical University, Szeged, 6701, Hung..
SOURCE: Planta Medica, (2000) Vol. 66, No. 3, pp. 291-294.
CODEN: PLMEAA. ISSN: 0032-0943.
COUNTRY: HUNGARY
DOCUMENT TYPE: Journal
FILE SEGMENT: CAPLUS
OTHER SOURCE: CAPLUS 2000:310802
LANGUAGE: English
ENTRY DATE: Entered STN: 20011116
Last Updated on STN: 20020326

AB From a pro-**inflammatory** active ext. of Euphorbia peplus, two new diterpene polyesters I and II based on the pepluane and jatrophane skeletons were isolated, together with four known **ingenane** and jatrophane diterpenes. The structures were detd. on the basis of extensive NMR studies. **Ingenol** 3-**angelate**, which was obtained for the first time from this plant, is an irritant toxin with high activity.

L34 ANSWER 3 OF 10 TOXCENTER COPYRIGHT 2002 ACS DUPLICATE 2
ACCESSION NUMBER: 1998:89050 TOXCENTER
COPYRIGHT: Copyright 2002 BIOSIS
DOCUMENT NUMBER: PREV199800394066
TITLE: Dietary **cancer** risk from conditional **cancerogens** in produce of livestock fed on species of spurge (Euphorbiaceae). III. Milk of lactating goats fed on the skin irritant herb Euphorbia peplus is polluted by **tumor** promoters of the **ingenane** diterpene ester type

AUTHOR(S): Zayed, Salah M. A. D.; Farghaly, Madiha; Taha, Hamdy; Gminski, Richard; Hecker, Erich (1)
CORPORATE SOURCE: (1) Deutsches Krebsforschungszentrum, Div. S0109, Res. Program 3, Risk Factors Cancer Cancer Prevention, In Neuenheimer Feld 280, D-69120 Heidelberg Germany
SOURCE: Journal of Cancer Research and Clinical Oncology, (June, 1998) Vol. 124, No. 6, pp. 301-306.
ISSN: 0171-5216.
DOCUMENT TYPE: Article
FILE SEGMENT: BIOSIS
OTHER SOURCE: BIOSIS 1998:394066
LANGUAGE: English
ENTRY DATE: Entered STN: 20011116
Last Updated on STN: 20011116

AB Special procedures were developed to investigate poisonous milk of lactating goats fed experimentally on aerial parts of the herb Euphorbia peplus L. In extracts of the milk, weakly irritant in the mouse-ear assay, three diterpene ester toxins were detected by techniques of high-performance liquid chromatography. They are of the **ingenane** structural type: Euphorbia factor Pel (**ingenol** 20-acetate 3-**angelate**), Euphorbia factor Pe2 (20-**deoxyingenol** 3-**angelate**) and Euphorbia factor Pe4 (20-**deoxyingenol** -6alpha,7alpha-epoxide 3-**angelate**). From goats milk collected 15 days after cessation of the experimental feeding period, extracts were completely free of diterpene ester toxins. The toxins polluting the milk are identical to diterpene ester entities occurring in the aerial parts of E. peplus. Of these, Euphorbia factors Pel and Pe2 are known as promoters of **tumors** of mouse skin. Apart from the toxic Euphorbia factors, the non-toxic parent alcohol **ingenol** was also detected in the milk. It is absent in the plant, and may have been generated metabolically from a certain portion of the toxic diterpene esters picked up by the goats from their fodder. The results presented here provide, for the first time, data for a novel interpretation of the locally high incidence of esophageal **cancer** observed in certain areas in the Caspian littoral of Iran, associated with a greater consumption of goat's (and sheep's) milk.

L34 ANSWER 4 OF 10 NAPRALERT COPYRIGHT (C) 2002 BD. TRUSTEES, U. IL.
ACCESSION NUMBER: 1998:6172 NAPRALERT
DOCUMENT NUMBER: J16371
TITLE: DIETARY **CANCER** RISK CONDITIONAL **CANCEROGENS** IN PRODUCE OF LIVESTOCK FED ON SPECIES OF SPURGE (EUPHORBIACEAE). I. SKIN IRRITANT AND **TUMOR** -PROMOTING **INGENANE**-TYPE DITERPENE ESTER IN E.PEPLUS, ONE OF SEVERAL HERBACEOUS EUPHORBIA SPECIES CONTAMINATING FODDER OF LIVESTOCK
AUTHOR: ZAYED S M A D; FARGHALY M; TAHA H; GOTTA H; HECKER E
CORPORATE SOURCE: LAB ORG CHEM, NATL RES CENT, CAIRO EGYPT
SOURCE: J CANCER RES CLIN ONCOL (1998) 124 (3/4) p. 131-140.
DOCUMENT TYPE: (Research paper)
LANGUAGE: ENGLISH
CHARACTER COUNT: 4068

L34 ANSWER 5 OF 10 TOXCENTER COPYRIGHT 2002 ACS DUPLICATE 3
ACCESSION NUMBER: 1985:140316 TOXCENTER
COPYRIGHT: Copyright 2002 ACS
DOCUMENT NUMBER: CA10319157302T
TITLE: Constituents of Egyptian Euphorbiaceae. Part 13. Biologically active diterpene esters from Euphorbia peplus
AUTHOR(S): Rizk, A. M.; Hammouda, F. M.; El-Missiry, M. M.; Radwan,

H. M.; Evans, F. J.
CORPORATE SOURCE: Pharm. Sci. Lab., Natl. Res. Cent., Cairo, Egypt.
SOURCE: Phytochemistry (Elsevier), (1985) Vol. 24, No. 7, pp. 1605-6.
CODEN: PYTCAS. ISSN: 0031-9422.
COUNTRY: EGYPT
DOCUMENT TYPE: Journal
FILE SEGMENT: CAPLUS
OTHER SOURCE: CAPLUS 1985:557302
LANGUAGE: English
ENTRY DATE: Entered STN: 20011116
Last Updated on STN: 20021112

AB By means of partition and preparative TLC, 2 pro-**inflammatory** diterpene esters were isolated from E. peplus. These compds. were identified as 20-**deoxyingenol** 3-O-**angelate**, which exhibited an irritant dose (for 50% irritation) of 0.18 .mu.g on mouse skin, and the new ester **ingenol** 20-O-octanoate (I), which exhibited an irritant dose (for 50% irritation) of 1.0 .mu.g on mouse skin.

L34 ANSWER 6 OF 10 TOXCENTER COPYRIGHT 2002 ACS DUPLICATE 4
ACCESSION NUMBER: 1983:65815 TOXCENTER
COPYRIGHT: Copyright 2002 BIOSIS
DOCUMENT NUMBER: BA75:15145
TITLE: **INGENOL** ESTERS FROM THE PRO **INFLAMMATORY** FRACTION OF EUPHORBIA-KAMERUNICA
AUTHOR(S): ABO K A; EVANS F J
CORPORATE SOURCE: DEP. PHARMACOGNOSY, SCH. PHARMACY, UNIV. LONDON, 29-39, BRUNSWICK SQUARE, LONDON, WC1N 1AX, UK.
SOURCE: PHYTOCHEMISTRY (OXF), (1982) 21 (3), 725-726
CODEN: PYTCAS. ISSN: 0031-9422.
FILE SEGMENT: BIOSIS
OTHER SOURCE: BIOSIS 1983:165145
LANGUAGE: English
ENTRY DATE: Entered STN: 20011116
Last Updated on STN: 20011116

AB A series of unstable mono- and diesters of the tetracyclic diterpene **ingenol** were isolated from the proinflammatory ether-soluble fraction of the latex of E. kamerunica. The esters were isolated by a neutral process involving column chromatography and TLC. The monoesters were identified by spectroscopic methods and hydrolysis reactions as **ingenol**-3-decanoate, **ingenol**-3-dodecanoate, **ingenol**-5-hexadienoate and **ingenol**-5-octenoate and the diesters as 20-acetyl-**ingenol**-3-octenoate and 20-acetyl-**ingenol**-3-**angelate**.

L34 ANSWER 7 OF 10 TOXCENTER COPYRIGHT 2002 ACS DUPLICATE 5
ACCESSION NUMBER: 1983:71571 TOXCENTER
COPYRIGHT: Copyright 2002 BIOSIS
DOCUMENT NUMBER: BA75:58451
TITLE: THE ACTIVE PRINCIPLES OF THE SPURGE FAMILY EUPHORBIACEAE 4. SKIN IRRITANT AND **TUMOR** PROMOTING DI TERPENE ESTERS FROM EUPHORBIA-INGENS
AUTHOR(S): OPFERKUCH H J; HECKER E
CORPORATE SOURCE: INST. BIOCHEM., DEUTSCHES KREBSFORSCHUNGSZENT., IM NEUENHEIMER FELD 280, D-6900 HEIDELBERG 1, W. GER.
SOURCE: J CANCER RES CLIN ONCOL, (1982) 103 (3), 255-268
CODEN: JCROD7. ISSN: 0171-5216.
FILE SEGMENT: BIOSIS
OTHER SOURCE: BIOSIS 1983:208451

LANGUAGE: English
ENTRY DATE: Entered STN: 20011116
Last Updated on STN: 20011116

AB The irritant and **tumor**-promoting principles of the latex of E. ingens E. Mey were isolated with several nonirritant compounds. The Euphorbia factors I1, I5 and I6 are esters of **ingenane**-type polyfunctional diterpene alcohols. Euphorbia factor I1 is characterized as the 3-hexadecanoate of the polyfunctional parent alcohol **ingenol** and Euphorbia factor I6 as the 3-deca-2.4.6-trienoic acid ester of **ingenol**. Euphorbia factor I5 is the 16-**angelate**-3-deca-2.4.6-trienoate of 16-**hydroxyingenol**. Nonirritant diterpenes of the latex are I2, the **ingenol** -2-hexadecanoate-an isomer of Euphorbia factor I1- and I4, the 3.7.12-triacetate-8-nicotinate of the macrocyclic lathyrane-type polyfunctional diterpene alcohol ingol. The diterpene alcohols **ingenol** and 16-**hydroxyingenol** are inactive as irritants and **tumor** promoters of mouse skin. Compared to croton oil factor A1 (TPA), the Euphorbia factor I1 exhibits about 1/10 of the irritant and **tumor**-promoting activity in mouse skin I1 shows no reasonable **tumorigenic** activity. Compared with I1, Euphorbia factors I5 and I6 are more potent irritants and less potent **tumor** promoters.

L34 ANSWER 8 OF 10 BABS COPYRIGHT 2002 BEILSTEIN CDS MDLI
ACCESSION NUMBER: 6235562 BABS
TITLE: Diterpenoids from Euphorbia peplus
AUTHOR(S): Hohmann, Judit; Evanics, Ferenc; Berta, Laszlo; Bartok, Tibor
SOURCE: Planta Med. (2000), 66(3), 291 - 294
CODEN: PLMEAA
DOCUMENT TYPE: Journal
LANGUAGE: English
SUMMARY LANGUAGE: English
AN 6235562 BABS
AB From a pro-**inflammatory** active extract of Euphorbia peplus, two new diterpene polyesters based on the pepluane and jatrophane skeletons were isolated, together with four known **ingenane** and jatrophane diterpenes. The structures were determined on the basis of extensive NMR studies. **Ingenol** 3-**angelate**, which was obtained for the first time from this plant, is an irritant toxin with high activity.

L34 ANSWER 9 OF 10 BABS COPYRIGHT 2002 BEILSTEIN CDS MDLI
ACCESSION NUMBER: 5865227 BABS
TITLE: BIOLOGICALLY ACTIVE DITERPENE ESTERS FROM EUPHORBIA PEPLUS
AUTHOR(S): Rizk, A. M.; Hammouda, F. M.; El-Missiry, M. M.; Radwan, H. M.; Evans, F. J.
SOURCE: Phytochemistry (1985), 24(7), 1605-1606
CODEN: PYTCAS
DOCUMENT TYPE: Journal
LANGUAGE: English
SUMMARY LANGUAGE: English
AN 5865227 BABS

L34 ANSWER 10 OF 10 BABS COPYRIGHT 2002 BEILSTEIN CDS MDLI
ACCESSION NUMBER: 5828746 BABS
TITLE: **INGENOL** ESTERS FROM THE PRO-**INFLAMMATORY** FRACTION OF EUPHORBIA KAMERUNICA
AUTHOR(S): Abo, Kio A.; Evans, Fred J.
SOURCE: Phytochemistry (1982), 21(3), 725-726

CODEN: PYTCAS
DOCUMENT TYPE: Journal
LANGUAGE: English
SUMMARY LANGUAGE: English
AN 5828746 BABS
AB A series of unstable mono- and di-esters of the tetracyclic diterpene **ingenol** were isolated from the pro-**inflammatory** ether-soluble fraction of the latex of Euphorbia kamerunica.The esters were isolated by a neutral process involving column and thin-layer chromatography.The monoesters were identified by spectroscopic methods and hydrolysis reactions as **ingenol**-3-decanoate, **ingenol** -3-dodecanoate, **ingenol**-5-hexadienoate and **ingenol** -5-octenoate and the diesters as 20-acetyl-**ingenol**-3-octenoate and 20-acetyl-**ingenol**-3-**angelate**.